



STIC Search Report

EIC 1700

STIC Database Tracking Number: 159797

TO: Rip A Lee
Location: REM 10A24
Art Unit : 1713
August 2, 2005

Case Serial Number: 10/673896

From: Usha Shrestha
Location: EIC 1700
REMSSEN 4B28
Phone: 571/272-3519
usha.shrestha@uspto.gov

Search Notes



STIC Search Results Feedback Form

EIC17000

Questions about the scope or the results of the search? Contact *the EIC searcher or contact:*

Kathleen Fuller, EIC 1700 Team Leader
571/272-2505 REMSEN 4B28

Voluntary Results Feedback Form

- I am an examiner in Workgroup: Example: 1713
➤ Relevant prior art **found**, search results used as follows:

- ☐ 102 rejection
- ☐ 103 rejection
- ☐ Cited as being of interest.
- ☐ Helped examiner better understand the invention.
- ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature
(journal articles, conference proceedings, new product announcements etc.)

➤ Relevant prior art **not found**:

- ☐ Results verified the lack of relevant prior art (helped determine patentability).
- ☐ Results were not useful in determining patentability or understanding the invention.

Comments:

Drop off or send completed forms to EIC1700 REMSEN 4B28



SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: LEE, R. A. Examiner #: 70600 Date: JULY 18, 2005
 Art Unit: 1713 Phone Number: 2-1104 Serial Number: 10/673,896
 Mail Box and Bldg/Room Location: REM 10A24 Results Format Preferred (circle): PAPER ☐ DISK ☐ E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

 Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: ZWITTERIONIC METALLOCYCLES

Inventors (please provide full names): NAGY, Sándor
MACK, Mark P.

SCIENTIFIC REFERENCE BR
 Sci & Tech Inf Ctr

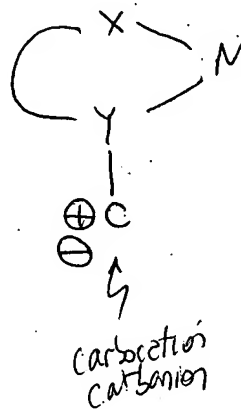
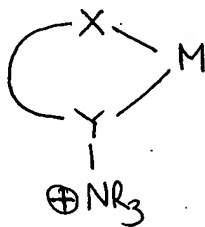
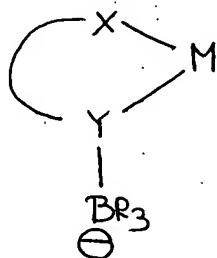
Earliest Priority Filing Date: SEPT-29-2003

JUL 19 RECD

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued parent numbers) along with the appropriate serial number.

Pat. & T.M. Office

Please search for compounds having the following structure



X, Y = N, O, P or S
 M = metal

STAFF USE ONLY

Type of Search

Vendors and cost where applicable

Searcher: _____

NA Sequence (#) _____

STN 396-1 426-11

Searcher Phone #: _____

AA Sequence (#) _____

Dialog _____

Searcher Location: _____

Structure (#) 3

Questel/Orbit _____

Date Searcher Picked Up: _____

Bibliographic _____

Dr. Link _____

Date Completed: _____

Litigation _____

Lexis/Nexis _____

Searcher Prep & Review Time: 90

Fulltext _____

Sequence Systems _____

Clerical Prep Time: 30

Patent Family _____

WWW/Internet _____

Online Time: 200

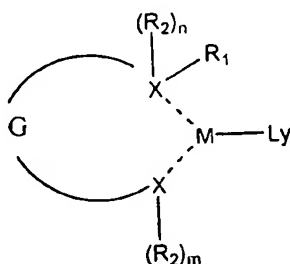
Other _____

Other (specify) _____

10/673,896

We claim:

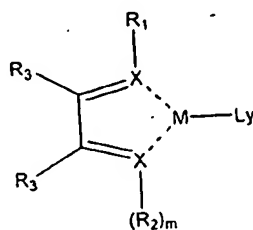
1. A zwitterionic metallocycle comprising a Group 4-10 transition metal chelated to two heteroatoms independently selected from the group consisting of P, N, O, and S wherein the two heteroatoms are each attached to a linking group to form a metallocycle and wherein one of the heteroatoms has a substituent bearing a full or partial negative charge and the transition metal has a full or partial positive charge.
2. The zwitterionic metallocycle of claim 1 wherein the substituent bears a negative charge on an atom selected from the group consisting of B, Al, Sn and Sb.
3. A zwitterionic metallocycle of general formula:



wherein M is a Group 4-10 transition metal bearing a full or partial positive charge, G is a linking group to form a metallocycle, each X is independently selected from the group consisting of P, N, O and S, each R_2 is independently selected from the group consisting of C_1 - C_{30} hydrocarbyl, m is 0, 1 or 2, n is 0 or 1, R_1 contains an atom bearing a full or partial negative charge selected from the group consisting of B, Al, Sn and Sb, L is independently selected from the group consisting of halide, alkoxy, siloxy, alkylamino, and C_1 - C_{30} hydrocarbyl and y satisfies the valence of M .

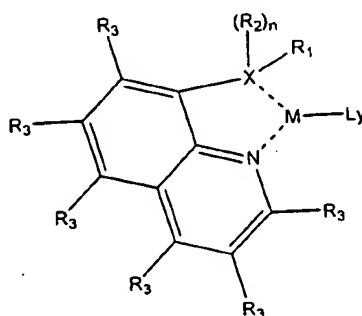
4. The zwitterionic metallocycle of claim 3 wherein G comprises two substituted or unsubstituted sp^2 carbon atoms to form a 5-membered metallocycle.

5. The zwitterionic metallocycle of claim 3 wherein X is N and R₁ contains an atom bearing a full or partial negative charge selected from the group consisting of B and Al.
6. The zwitterionic metallocycle of claim 4 having the general formula:



wherein each R₃ is independently selected from the group consisting of H and C₁-C₃₀ hydrocarbyl and m is 0 or 1.

7. The zwitterionic metallocycle of claim 4 having the general formula:



wherein each R₃ is independently selected from the group consisting of H and C₁-C₃₀ hydrocarbyl.

8. An olefin polymerization process comprising contacting an olefin with a zwitterionic metallocycle comprising a Group 4-10 transition metal chelated to two heteroatoms independently selected from the group consisting of P, N, O, and S wherein the two heteroatoms are each attached to a linking group to form a metallocycle, and wherein one of the heteroatoms has a

=> d his

FILE 'REGISTRY' ENTERED AT 08:32:20 ON 02 AUG 2005
ACT LEE896/A

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L1      STR
L2      SCR 2040
L3      SCR 1964 OR 1921 OR 1931
L4      90718 SEA FILE=REGISTRY SSS FUL L1 AND L2 AND L3

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FILE 'HCAPLUS' ENTERED AT 08:46:49 ON 02 AUG 2005

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L5      23969 S L4
L6      2064 S L5 (L) CAT/RL
L7      517 S L6 AND (POLYMER? OR PLASTIC?)/SC
L8      1 S US20050070728/PN
L9      1 S L7 AND L8
L10     3 S L7 AND ZWITTER?
L11     415 S L6 (L) POLYMERI?
L12     340 S L11 AND (POLYMER? OR PLASTIC?)/SC
L13     234 S L6 (L) POLYMERI? (2A) CATALYST?
L14     128 S L13 (L) PREP/RL
L15     103 S L14 AND (POLYMER? OR PLASTIC?)/SC
L16     89 S L5 AND ZWITTER?
L17     13 S L16 AND CAT/RL

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FILE 'REGISTRY' ENTERED AT 09:07:32 ON 02 AUG 2005

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L18     STR L1
L19     STR L18
L20     12 S (L18 OR L19) SAM SUB=L4
L21     751 S (L18 OR L19) FUL SUB=L4
        SAV L21 LEE1896/A

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FILE 'HCAPLUS' ENTERED AT 09:29:01 ON 02 AUG 2005

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L22     190 S L21
L23     0 S L22 AND L8
L24     3 S L22 (L) CAT/RL
L25     3 S L22 AND CAT/RL
L26     5 S L22 AND CATALY?
L27     0 S L15 AND ZWITTER?
L28     18 S L10 OR L17 OR L24 OR L25 OR L26

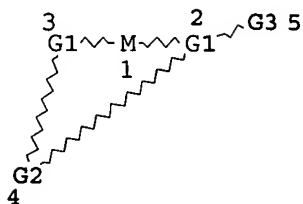
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=> d que 15

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L1      STR

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VAR G1=O/S/N/P
REP G2=(2-3) C
VAR G3=B/N/C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

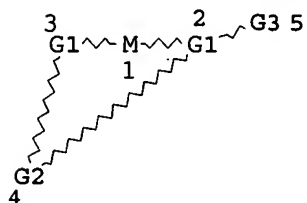
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NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE

L2 SCR 2040
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L4 90718 SEA FILE=REGISTRY SSS FUL L1 AND L2 AND L3
L5 23969 SEA FILE=HCAPLUS ABB=ON PLU=ON L4

=> d que 122

L1 STR



VAR G1=O/S/N/P

REP G2=(2-3) C

VAR G3=B/N/C

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

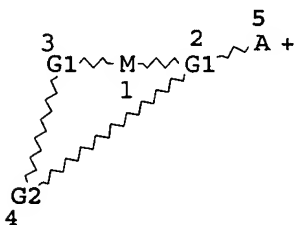
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE

L2 SCR 2040
L3 SCR 1964 OR 1921 OR 1931
L4 90718 SEA FILE=REGISTRY SSS FUL L1 AND L2 AND L3
L18 STR



VAR G1=O/S/N/P

REP G2=(2-3) C

NODE ATTRIBUTES:

CHARGE IS *+ AT 5

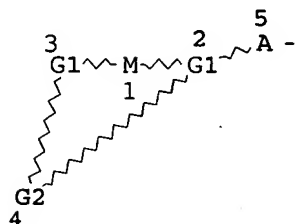
DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE
L19 STR



VAR G1=O/S/N/P
REP G2=(2-3) C
NODE ATTRIBUTES:
CHARGE IS *- AT 5
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE
L21 751 SEA FILE=REGISTRY SUB=L4 SSS FUL (L18 OR L19)
L22 190 SEA FILE=HCAPLUS ABB=ON PLU=ON L21

=> fil hcap
FILE 'HCAPLUS' ENTERED AT 10:05:53 ON 02 AUG 2005

=> d l28 1-18 ibib abs hitstr hitind

L28 ANSWER 1 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:283221 HCAPLUS
DOCUMENT NUMBER: 142:336805
TITLE: **Zwitterionic** metallocycles for
olefin polymerizations
INVENTOR(S): Nagy, Sandor; Mack, Mark P.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 7 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 2005070728	A1	20050331	US 2003-673896	2003 0929
WO 2005033154	A1	20050414	WO 2004-US28992	2004 0907

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ,

CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG,
 ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP,
 KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD,
 MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL,
 PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR,
 TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM,
 ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH,
 CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU,
 MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI,
 CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2003-673896

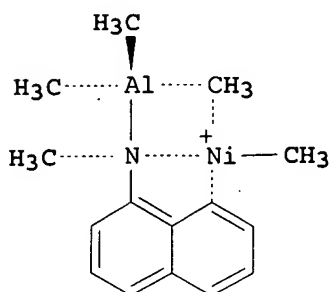
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2003
 0929

OTHER SOURCE(S):

MARPAT 142:336805

GI



I

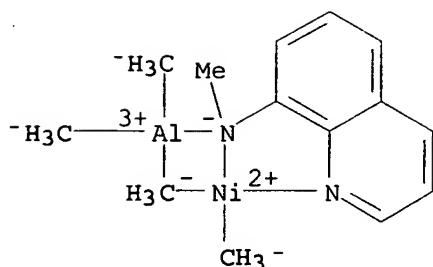
AB Title **zwitterionic** metallocycle comprises a Group 4-10 transition metal chelated to two heteroatoms independently selected from the group consisting of P, N, O, and S (e.g., I), wherein the two heteroatoms are each attached to a linking group to form a metallocycle and wherein one of the heteroatoms has a substituent bearing a full or partial neg. charge and the transition metal has a full or partial pos. charge. We have found that substitution in this position stabilizes the **zwitterion** form of the metallocycle. The **zwitterionic** metallocycle is useful for olefin polymns (e.g., polyethylene).

IT 848644-67-7P 848644-68-8P

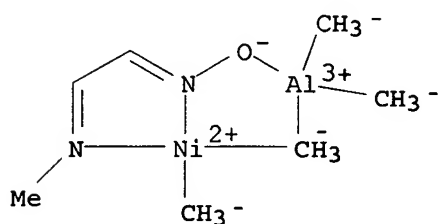
(production of **zwitterionic** metallocycles for olefin polymns.)

RN 848644-67-7 HCAPLUS

CN INDEX NAME NOT YET ASSIGNED



RN 848644-68-8 HCAPLUS
 CN INDEX NAME NOT YET ASSIGNED



IC ICM C07F009-00
 ICS C07F017-00; C07F013-00
 INCL 556013000; 556046000; 556043000; 556140000
 CC 35-3 (Chemistry of Synthetic High Polymers)
 Section cross-reference(s): 29, 67
 ST **zwitterionic** metallocycle olefin polymn polyethylene
 IT Polymerization
 (gas-phase; production of **zwitterionic** metallocycles for
 olefin polymns.)
 IT Polymerization catalysts
 (metallacycles; production of **zwitterionic** metallocycles
 for olefin polymns.)
 IT Metallacycles
 (polymerization catalyst; production of **zwitterionic**
 metallocycles for olefin polymns.)
 IT **Zwitterions**
 (production of **zwitterionic** metallocycles for olefin
 polymns.)
 IT Polymerization
 (slurry; production of **zwitterionic** metallocycles for
 olefin polymns.)
 IT 75-24-1, Trimethyl aluminum
 (production of **zwitterionic** metallocycles for olefin
 polymns.)
 IT **848644-67-7P 848644-68-8P**
 (production of **zwitterionic** metallocycles for olefin
 polymns.)
 IT 9002-88-4P, Polyethylene
 (production of **zwitterionic** metallocycles for olefin
 polymns.)
 IT 7718-54-9, Nickel dichloride, reactions 14148-44-8,
 8-(Methylamino)quinoline 848573-24-0
 (starting material; production of **zwitterionic**

metallocycles for olefin polymns.)

L28 ANSWER 2 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:807665 HCAPLUS

DOCUMENT NUMBER: 142:6639

TITLE: Stepwise Synthesis, Structures, and Reactivity of Mono-, Di-, and Trimetallic Metal Complexes with a $6\pi + 6\pi$ Quinonoid Zwitterion

AUTHOR(S): Taquet, Jean-Philippe; Siri, Olivier; Braunstein, Pierre; Welter, Richard

CORPORATE SOURCE: Laboratoire de Chimie de Coordination and Laboratoire DECMET UMR 7513 CNRS, Universite Louis Pasteur, Strasbourg, F-67070, Fr.

SOURCE: Inorganic Chemistry (2004), 43(22), 6944-6953
CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

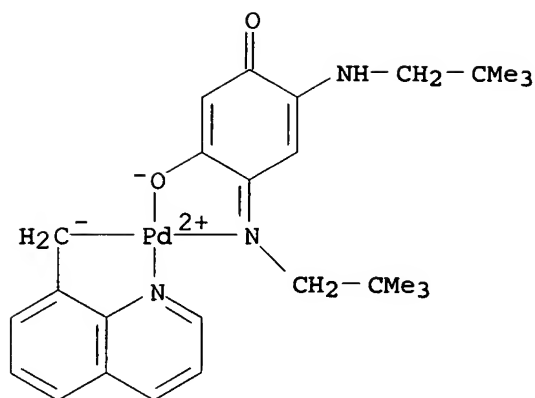
AB The benzoquinone monoimine N,N'-dineopentyl-2-amino-5-alcoholate-1,4-benzoquinonemonoiminium [C₆H₂(NHCH₂tBu)₂(O)₂] (6), which is a rare example of an organic zwitterion being more stable than its canonical form, is best described as constituted of two chemical connected but electronically not conjugated 6π electron subunits. The two successive acidities of 6 gave mono-, di-, and trimetallic complexes in which the control of the π -system delocalization becomes possible. Reaction of 6 with NaOBu-t results in monodeprotonation of one N-H function, and the isolated Na salt (9), which is stable under N₂, reacts with chloride-bridged Pd(II) homodimetallic complexes, [AuCl(PPh₃)] or trans-[NiCl(Ph)(PPh₃)₂], to afford the monometallic complexes 10-15 in which the π -system is localized. A 2nd in situ deprotonation of the remaining N-H amino function of Pd complex 10 with NaH followed by reaction with [Pd(8-mq)(μ -Cl)]₂ (8-mq = orthometalated 8-methylquinoline) affords the homodimetallic complex (17) in which the π -system of the quinonoid ligand is delocalized between the two metal centers. Deprotonation of both N-H amino functions of the square-planar complex trans-[Ni(N,O)₂] (15; N,O = 4-neopentylamino-2-neopentylimino-5-oxocyclohexa-1,4-dienolato) with NaH and reaction with [Pd(8-mq)(μ -Cl)]₂ affords the heterotrimetallic (Pd, Ni, Pd) complex (18) in which the π -system of the two quinonoid ligands is delocalized between the three metal centers. The crystal structures of the monometallic complexes 10 and 13 and of the dipalladium complex 17 are reported and consequences of metal coordination discussed. Complex 15 was tested in catalytic ethylene oligomerization with AlEtCl₂ as cocatalyst.

IT 797816-73-0P 797816-76-3P

(crystal structure, fluxionality; preparation, crystal structure and reactions of gold, nickel and/or palladium amino(imino)oxocyclohexadienolato complexes)

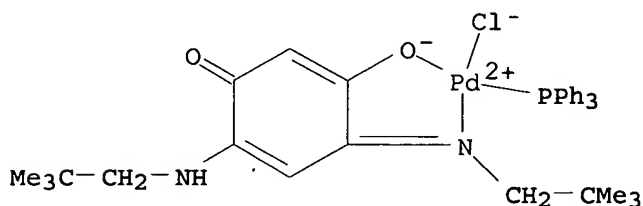
RN 797816-73-0 HCAPLUS

CN Palladium, [2-[(2,2-dimethylpropyl)amino]-4-[(2,2-dimethylpropyl)imino- κ N]-5-(hydroxy- κ O)-2,5-cyclohexadien-1-onato][(8-quinolinyl- κ N)methyl- κ C]-, (SP-4-4) - (9CI) (CA INDEX NAME)



RN 797816-76-3 HCAPLUS

CN Palladium, chloro[2-[(2,2-dimethylpropyl)amino]-4-[(2,2-dimethylpropyl)imino-κN]-5-(hydroxy-κO)-2,5-cyclohexadien-1-onato](triphenylphosphine)-, (SP-4-3)-(9CI) (CA INDEX NAME)



IT 798569-03-6P

(crystal structure; preparation, crystal structure and reactions of gold, nickel and/or palladium amino(imino)oxocyclohexadienolato complexes)

RN 798569-03-6 HCAPLUS

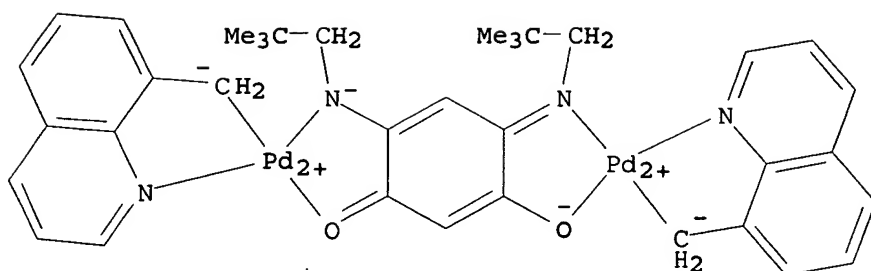
CN Palladium, [μ-[2-[(2,2-dimethylpropyl)amino-κN]-4-[(2,2-dimethylpropyl)imino-κN]-5-(hydroxy-κO)-2,5-cyclohexadien-1-onato(2-)-κO]]bis[(8-quinolinyl-κN)methyl-κC]di-, stereoisomer, compd. with tetrahydrofuran (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 797816-78-5

CMF C36 H40 N4 O2 Pd2

CCI CCS



CM 2

CRN 109-99-9

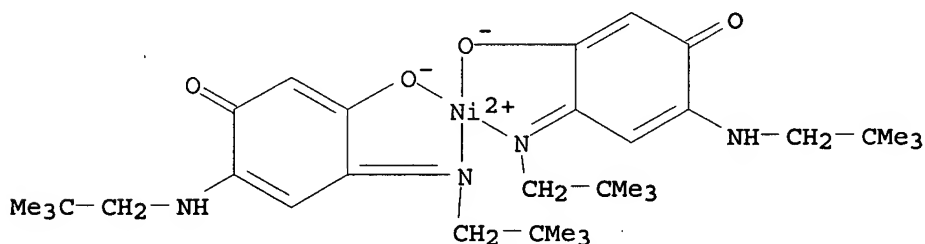
CMF C4 H8 O



IT 622784-51-4P, Bis[4-(neopentylamino)-2-(neopentylimino)-5-oxo-1,4-cyclohexadienolato]nickel
 (deprotonation followed by reaction with palladium complex; preparation, crystal structure and reactions of gold, nickel and/or palladium amino(imino)oxocyclohexadienolato complexes)

RN 622784-51-4 HCAPLUS

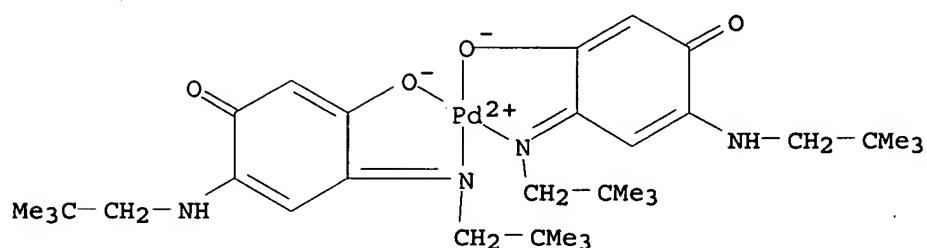
CN Nickel, bis[2-[(2,2-dimethylpropyl)amino]-4-[(2,2-dimethylpropyl)imino-κN]-5-(hydroxy-κO)-2,5-cyclohexadien-1-onato]- (9CI) (CA INDEX NAME)



IT 622784-54-7P, Bis[4-(neopentylamino)-2-(neopentylimino)-5-oxocyclohexa-1,4-dienolato]palladium
 (deprotonation followed by reaction with palladium complex; preparation, crystal structure and reactions of gold, nickel and/or palladium amino(imino)oxocyclohexadienolato complexes)

RN 622784-54-7 HCAPLUS

CN Palladium, bis[2-[(2,2-dimethylpropyl)amino]-4-[(2,2-dimethylpropyl)imino-κN]-5-(hydroxy-κO)-2,5-cyclohexadien-1-onato]- (9CI) (CA INDEX NAME)

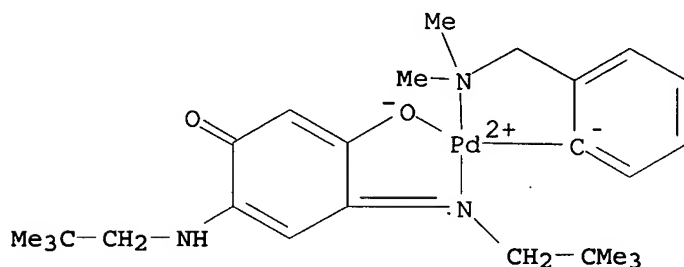


IT 797816-74-1P

(fluxionality; preparation, crystal structure and reactions of gold, nickel and/or palladium amino(imino)oxocyclohexadienolato complexes)

RN 797816-74-1 HCAPLUS

CN Palladium, [2-[(dimethylamino-κN)methyl]phenyl-κC][2-[(2,2-dimethylpropyl)amino]-4-[(2,2-dimethylpropyl)imino-κN]-5-(hydroxy-κO)-2,5-cyclohexadien-1-onato]-, (SP-4-4) - (9CI)
(CA INDEX NAME)

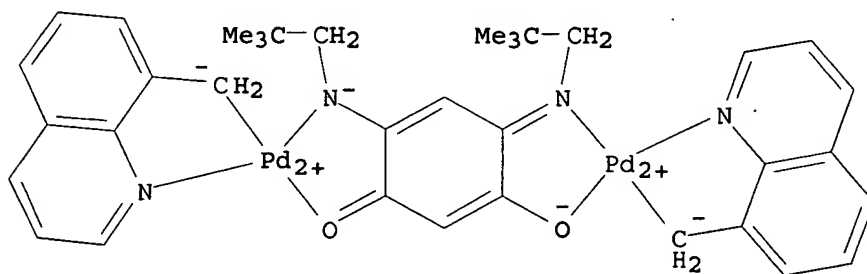


IT 797816-78-5P

(mol. structure, fluxionality; preparation, crystal structure and reactions of gold, nickel and/or palladium amino(imino)oxocyclohexadienolato complexes)

RN 797816-78-5 HCAPLUS

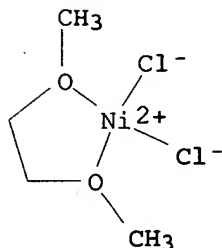
CN Palladium, [μ-[2-[(2,2-dimethylpropyl)amino-κN]-4-[(2,2-dimethylpropyl)imino-κN]-5-(hydroxy-κO)-2,5-cyclohexadien-1-onato(2-)-κO]]bis[(8-quinolinyl-κN)methyl-κC]di-, stereoisomer (9CI) (CA INDEX NAME)



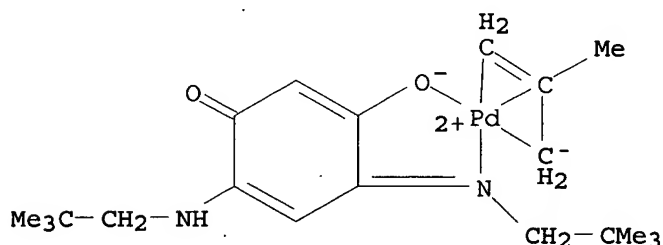
IT 29046-78-4, Dichloro(1,2-dimethoxyethane)nickel

(preparation, crystal structure and reactions of gold, nickel and/or

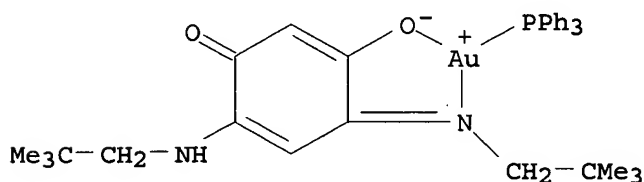
palladium amino(imino)oxocyclohexadienolato complexes)
 RN 29046-78-4 HCAPLUS
 CN Nickel, dichloro[1,2-di(methoxy- κ O)ethane] - (9CI) (CA INDEX NAME)



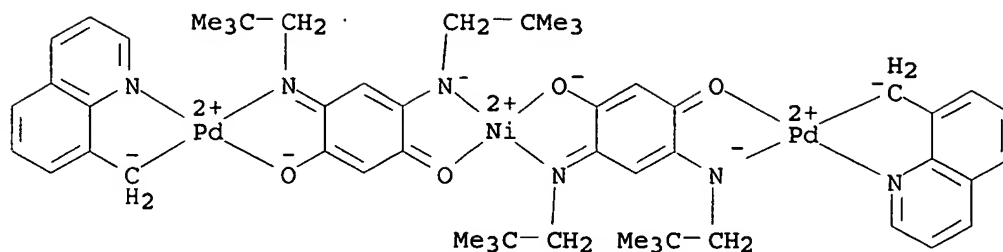
IT 797816-75-2P 797816-77-4P 797816-79-6P
 (preparation, crystal structure and reactions of gold, nickel and/or
 palladium amino(imino)oxocyclohexadienolato complexes)
 RN 797816-75-2 HCAPLUS
 CN Palladium, [2-[(2,2-dimethylpropyl)amino]-4-[(2,2-dimethylpropyl)imino- κ N]-5-(hydroxy- κ O)-2,5-cyclohexadien-1-onato] [(1,2,3- η)-2-methyl-2-propenyl] - (9CI)
 (CA INDEX NAME)



RN 797816-77-4 HCAPLUS
 CN Gold, [2-[(2,2-dimethylpropyl)amino]-4-[(2,2-dimethylpropyl)imino- κ N]-5-(hydroxy- κ O)-2,5-cyclohexadien-1-onato] (triphenylphosphine) - (9CI) (CA INDEX NAME)



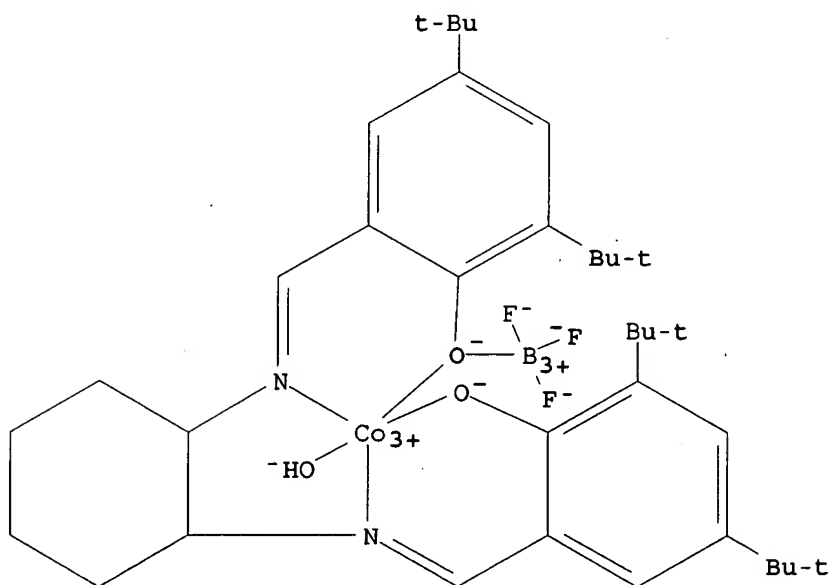
RN 797816-79-6 HCAPLUS
 CN Palladium, bis[μ -[2-[(2,2-dimethylpropyl)amino- κ N]-4-[(2,2-dimethylpropyl)imino- κ N]-5-(hydroxy- κ O)-2,5-cyclohexadien-1-onato(2-)- κ O]] (nickel) bis[(8-quinolinyl- κ N)methyl- κ C]di- (9CI) (CA INDEX NAME)



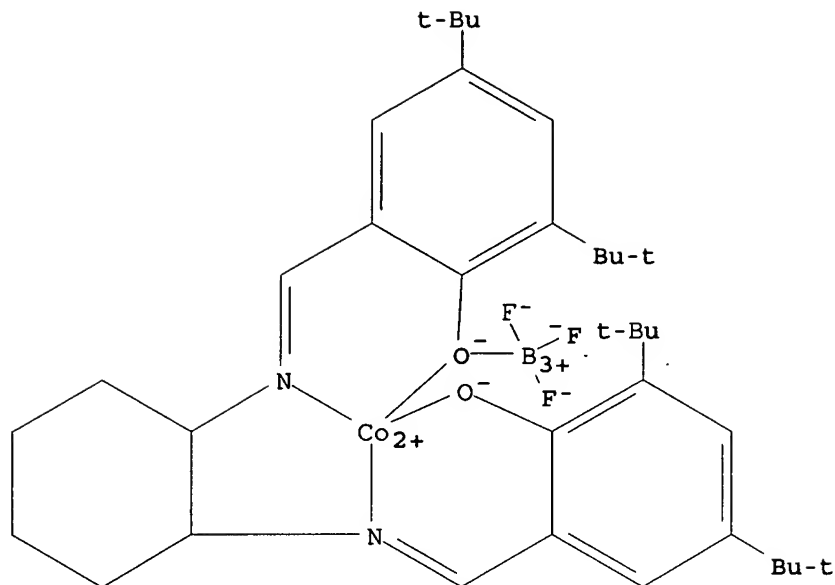
- CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 35, 75, 78
- IT 797816-73-0P 797816-76-3P
(crystal structure, fluxionality; preparation, crystal structure and reactions of gold, nickel and/or palladium amino(imino)oxocyclohexadienolato complexes)
- IT 798569-03-6P
(crystal structure; preparation, crystal structure and reactions of gold, nickel and/or palladium amino(imino)oxocyclohexadienolato complexes)
- IT 622784-51-4P, Bis[4-(neopentylamino)-2-(neopentylimino)-5-oxo-1,4-cyclohexadienolato]nickel
(deprotonation followed by reaction with palladium complex; preparation, crystal structure and reactions of gold, nickel and/or palladium amino(imino)oxocyclohexadienolato complexes)
- IT 622784-54-7P, Bis[4-(neopentylamino)-2-(neopentylimino)-5-oxocyclohexa-1,4-dienolato]palladium
(deprotonation followed by reaction with palladium complex; preparation, crystal structure and reactions of gold, nickel and/or palladium amino(imino)oxocyclohexadienolato complexes)
- IT 797816-74-1P
(fluxionality; preparation, crystal structure and reactions of gold, nickel and/or palladium amino(imino)oxocyclohexadienolato complexes)
- IT 797816-78-5P
(mol. structure, fluxionality; preparation, crystal structure and reactions of gold, nickel and/or palladium amino(imino)oxocyclohexadienolato complexes)
- IT 12081-18-4, Bis[(μ-chloro)(η³-2-methylallyl)palladium]
14243-64-2, Chloro(triphenylphosphine)gold 14873-91-7,
Dichlorobis(ethanethiolato)palladium 15134-30-2 18987-59-2,
Bis[(μ-chloro)[2-[(dimethylamino)methyl]phenyl]palladium]
28377-73-3, Bis[(μ-chloro)[(quinolin-8-yl)methyl]palladium]
29046-78-4, Dichloro(1,2-dimethoxyethane)nickel
33571-43-6, trans-Chloro(phenyl)bis(triphenylphosphine)nickel
67756-93-8 67773-32-4
(preparation, crystal structure and reactions of gold, nickel and/or palladium amino(imino)oxocyclohexadienolato complexes)
- IT 797816-75-2P 797816-77-4P 797816-79-6P
(preparation, crystal structure and reactions of gold, nickel and/or palladium amino(imino)oxocyclohexadienolato complexes)
- REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L28 ANSWER 3 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:744997 HCAPLUS
DOCUMENT NUMBER: 141:410760
TITLE: New chiral cobalt salen complexes containing

Lewis acid BF_3 ; a highly reactive and enantioselective **catalyst** for the hydrolytic kinetic resolution of epoxides
 AUTHOR(S): Shin, Chang-Kyo; Kim, Seong-Jin; Kim, Geon-Joong
 CORPORATE SOURCE: Department of Chemical Engineering, Inha University, Inchon, 402-751, S. Korea
 SOURCE: Tetrahedron Letters (2004), 45(40), 7429-7433
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 141:410760
 AB A new type of chiral cobalt salen complexes bearing BF_3 Lewis acid proved to be reactive and enantioselective in the hydrolytic resolution of terminal epoxides. The polymer type salen **catalysts** also showed a high enantioselectivity in the same reaction.
 IT 792956-29-7P 792956-31-1P
 (chiral cobalt salen complexes containing Lewis acid BF_3 as **catalysts** for the kinetic resolution of epoxides)
 RN 792956-29-7 HCAPLUS
 CN Cobalt, [[2-[[[(1R,2R)-2-[[[3,5-bis(1,1-dimethylethyl)-2-hydroxyphenyl]methylene]amino]cyclohexyl]imino]methyl]-4,6-bis(1,1-dimethylethyl)phenolato(2-)- κO]trifluoroborato(2-)- $\kappa\text{N},\kappa\text{N}',\kappa\text{O},\kappa\text{O}'$]hydroxy-, (SP-5-35)- (9CI)
 (CA INDEX NAME)



RN 792956-31-1 HCAPLUS
 CN Cobalt, [[2-[[[(1R,2R)-2-[[[3,5-bis(1,1-dimethylethyl)-2-hydroxyphenyl]methylene]amino]cyclohexyl]imino]methyl]-4,6-bis(1,1-dimethylethyl)phenolato(2-)- κO]trifluoroborato(2-)- $\kappa\text{N},\kappa\text{N}',\kappa\text{O},\kappa\text{O}'$]-, (SP-4-4)- (9CI) (CA INDEX NAME)



IT 792956-35-5P 792956-37-7P

(chiral cobalt salen complexes containing Lewis acid BF₃ as catalysts for the kinetic resolution of epoxides)

RN 792956-35-5 HCAPLUS

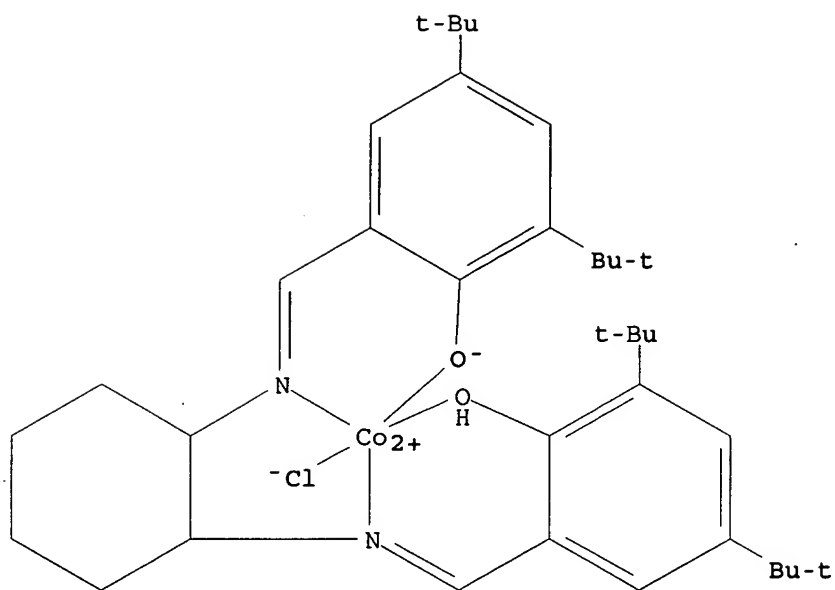
CN Cobalt, [[2-[[[(1R,2R)-2-[[[3,5-bis(1,1-dimethylethyl)-2-hydroxyphenyl]methylene]amino]cyclohexyl]imino]methyl]-4,6-bis(1,1-dimethylethyl)phenolato(2-)-κO]trifluoroborato(2-)-κN,κN',κO,κO']-, (SP-4-4)-, compd. with (SP-5-15)-[[[(1R,2R)-2,2'-[1,2-cyclohexanediylbis[(nitrilo-κN)methylidyne]]bis[4,6-bis(1,1-dimethylethyl)phenolato-κO]](1-)]chlorocobalt (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 792956-33-3

CMF C36 H53 Cl Co N2 O2

CCI CCS

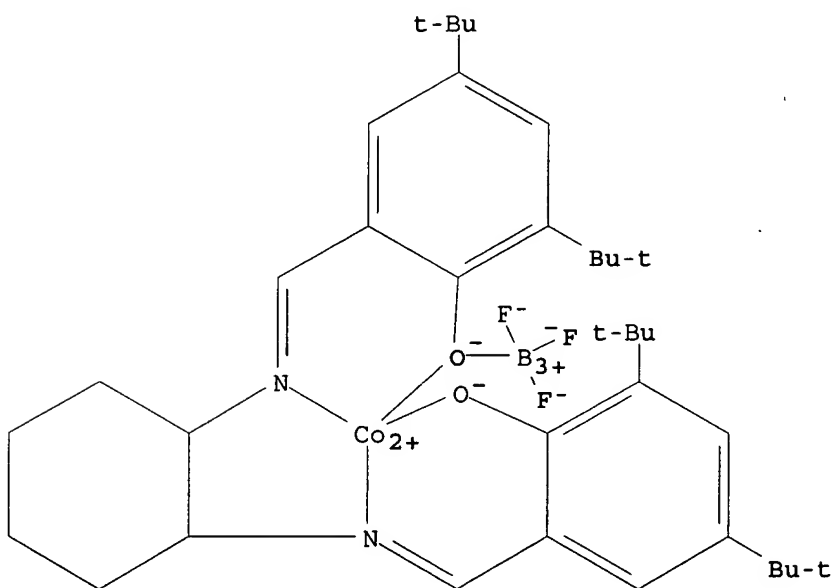


CM 2

CRN 792956-31-1

CMF C36 H52 B Co F3 N2 O2

CCI CCS



RN 792956-37-7 HCAPLUS

CN Cobalt, [[2-[[[(1R,2R)-2-[[[3,5-bis(1,1-dimethylethyl)-2-hydroxyphenyl]methylene]amino]cyclohexyl]imino]methyl]-4,6-bis(1,1-dimethylethyl)phenolato(2-)-κO]trifluoroborato(2-)-κN,κN',κO,κO']hydroxy-, (SP-5-35)-, compd.

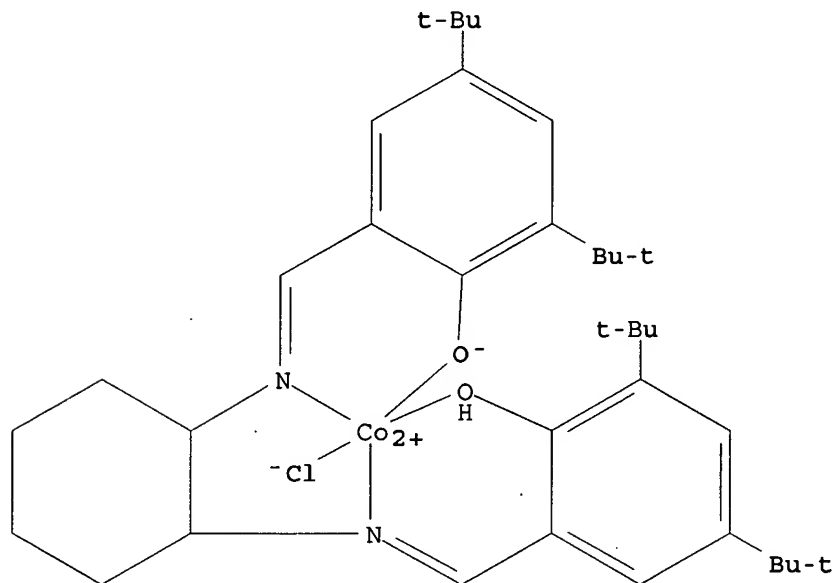
with (SP-5-15)-chloro[[2,2'-[(1R,2R)-1,2-cyclohexanediylbis[(nitrilo-κN)methylidyne]]bis[4,6-bis(1,1-dimethylethyl)phenolato-κO]](1-)]cobalt (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 792956-33-3

CMF C36 H53 Cl Co N2 O2

CCI CCS

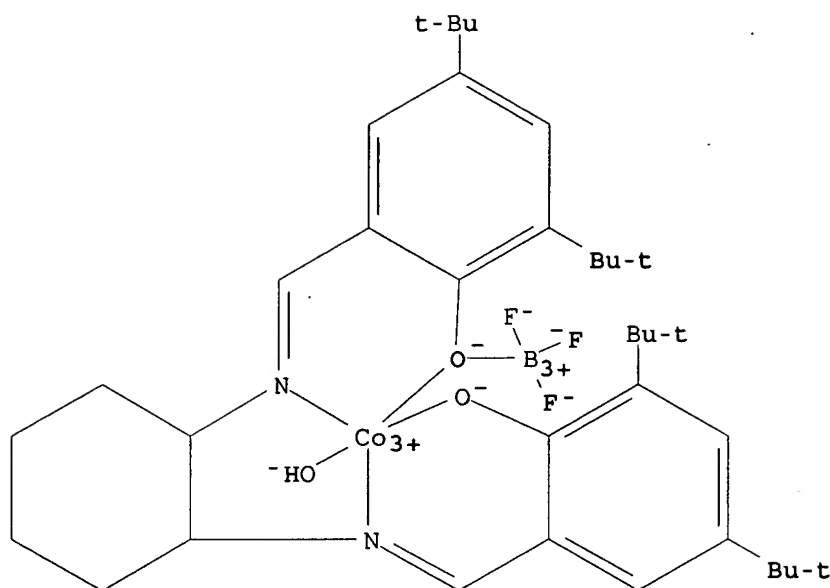


CM 2

CRN 792956-29-7

CMF C36 H53 B Co F3 N2 O3

CCI CCS



- CC 27-2 (Heterocyclic Compounds (One Hetero Atom))
 ST epoxide kinetic resolu chiral cobalt boron trifluoride
 catalyst
 IT Hydrolysis
 Hydrolysis catalysts
 (chiral cobalt salen complexes containing Lewis acid BF₃ as
 catalysts for the kinetic resolution of epoxides)
 IT Epoxides
 (chiral cobalt salen complexes containing Lewis acid BF₃ as
 catalysts for the kinetic resolution of epoxides)
 IT Alcohols, preparation
 (chiral cobalt salen complexes containing Lewis acid BF₃ as
 catalysts for the kinetic resolution of epoxides)
 IT Resolution (separation)
 (kinetic; chiral cobalt salen complexes containing Lewis acid BF₃
 as catalysts for the kinetic resolution of epoxides)
 IT 790672-70-7DP, cobalt complexes 792956-29-7P
 792956-31-1P
 (chiral cobalt salen complexes containing Lewis acid BF₃ as
 catalysts for the kinetic resolution of epoxides)
 IT 7440-48-4DP, Cobalt, complexes with chiral salen polymers
 792956-35-5P 792956-37-7P
 (chiral cobalt salen complexes containing Lewis acid BF₃ as
 catalysts for the kinetic resolution of epoxides)
 IT 3760-95-0P, (R)-Ethylloxirane 15448-47-2P, (R)-Methyloxirane,
 preparation 20780-53-4P, (R)-Styrene oxide 67843-74-7P,
 preparation
 (chiral cobalt salen complexes containing Lewis acid BF₃ as
 catalysts for the kinetic resolution of epoxides)
 IT 75-56-9, Propylene oxide, reactions 96-09-3, Styrene oxide
 106-88-7, 1,2-Epoxybutane 106-89-8, Epichlorohydrin, reactions
 176763-62-5 790672-69-4D, cobalt complexes
 (chiral cobalt salen complexes containing Lewis acid BF₃ as
 catalysts for the kinetic resolution of epoxides)
 IT 792956-33-3P
 (chiral cobalt salen complexes containing Lewis acid BF₃ as

catalysts for the kinetic resolution of epoxides)
 IT 4254-15-3P, (S)-1,2-Propanediol, preparation 25779-13-9P,
 (S)-1-Phenyl-1,2-ethanediol 57090-45-6P 73522-17-5P,
 (S)-1,2-Butanediol
 (chiral cobalt salen complexes containing Lewis acid BF₃ as
 catalysts for the kinetic resolution of epoxides)
 REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L28 ANSWER 4 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:181540 HCAPLUS

DOCUMENT NUMBER: 141:23695

TITLE: Synthesis, characterization and ethylene
 reactivity of 2-diphenylphosphanylbenzamido
 nickel complexes

AUTHOR(S): Kwon, Heon Yong; Lee, Su Yeon; Lee, Bun Yeoul;
 Shin, Dong Mok; Chung, Young Keun

CORPORATE SOURCE: Department of Molecular Science and
 Technology, Ajou University, Suwon, 442-749,
 S. Korea

SOURCE: Dalton Transactions (2004), (6), 921-928

CODEN: DTARAF; ISSN: 1477-9226

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:23695

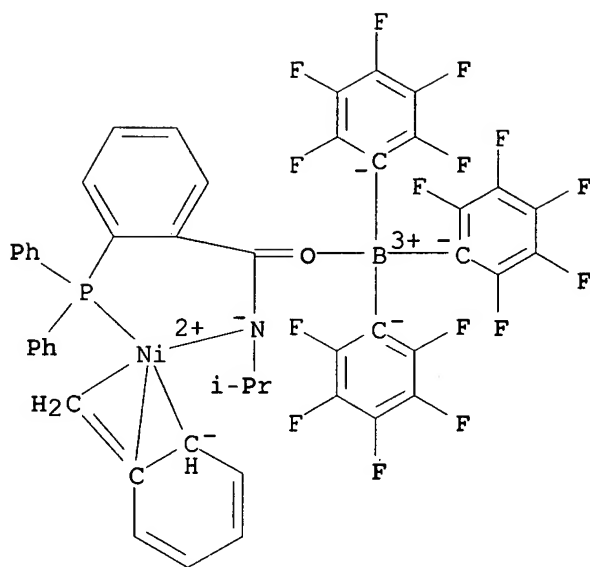
AB Addition of primary amines to N-[2-(diphenylphosphinyl)benzoyloxy]suc-
 cinimide affords 2-diphenylphosphinylbenzamides, Ph₂PC₆H₄C(O)NHR
 (R = C(CH₃)₃, 3; R = H, 4; R = CH₂CH₂CH₃, 5; R = CH(CH₃)₂, 6).
 Addition of NiCl(η³-CH₂C₆H₅)(PMe₃) to the deprotonated potassium
 salts of the amides and subsequent treatment with two equivalent of
 B(C₆F₅)₃ to the resulting products furnishes η³-benzyl
 zwitterionic nickel(II) complexes, [Ph₂PC₆H₄C(O)NR-
 κ²N,P]Ni(η³-CH₂C₆H₅) (R = C₆H₅, 9; R = C(CH₃)₃, 10; R =
 H, 11; R = CH₂CH₂CH₃, 12; R = CH(CH₃)₂, 13). Solid structures of
 9, 11, 13 and the intermediate η¹-benzyl nickel(II) complexes,
 [Ph₂PC₆H₄C(O)NR-κ²N,P]Ni(η¹-CH₂C₆H₅)(PMe₃) (R = C₆H₅, 7;
 R = C(CH₃)₃, 8) were determined by x-ray crystallog. When ethylene is
 added to the η³-benzyl zwitterionic nickel(II)
 complexes, butene is obtained from the complexes 9-12 but complex
 13 provides very high mol. weight branched polyethylene (Mw,
 .apprx.1,300,000) with excellent activity (up to 5, 200 kg mol⁻¹
 h⁻¹ at 100 psi gauge).

IT 697288-97-4P

(crystal structure; preparation, crystal structure, and catalytic
 activity of (diphenylphosphinyl)benzamido nickel complexes)

RN 697288-97-4 HCAPLUS

CN Nickel, [μ-[2-(diphenylphosphino-κP)-N-(1-
 methylethyl)benzamido-κN:κO]](η³-6-methylene-2,4-
 cyclohexadien-1-yl) [tris(pentafluorophenyl)boron]-, stereoisomer
 (9CI) (CA INDEX NAME)



IT 697289-03-5P
(crystal structure; preparation, crystal structure, and catalytic activity of (diphenylphosphinyl)benzamido nickel complexes)

RN 697289-03-5 HCAPLUS

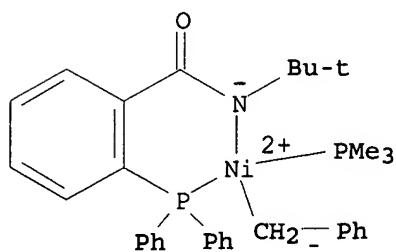
CN Nickel, [N-(1,1-dimethylethyl)-2-(diphenylphosphino- κ P)benzamido- κ N] (phenylmethyl) (trimethylphosphine)-, (SP-4-2)-, compd. with benzene (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 697288-92-9

CMF C33 H39 N Ni O P2

CCI CCS



CM 2

CRN 71-43-2

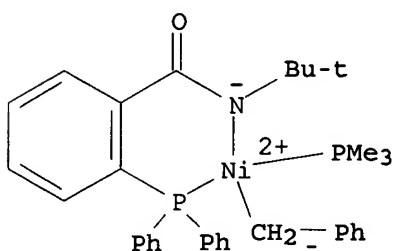
CMF C6 H6



IT 697288-92-9P

(mol. structure; preparation, crystal structure, and catalytic activity of (diphenylphosphinyl)benzamido nickel complexes)

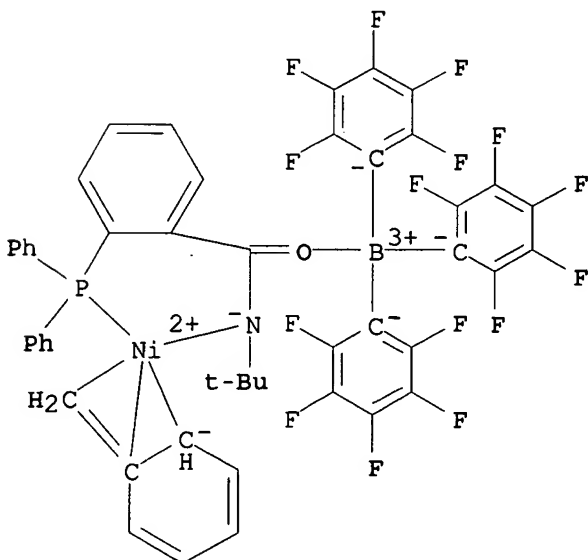
RN 697288-92-9 HCAPLUS

CN Nickel, [N-(1,1-dimethylethyl)-2-(diphenylphosphino- κ P)benzamido- κ N] (phenylmethyl) (trimethylphosphine)-, (SP-4-2)- (9CI) (CA INDEX NAME)

IT 697288-94-1P 697288-96-3P

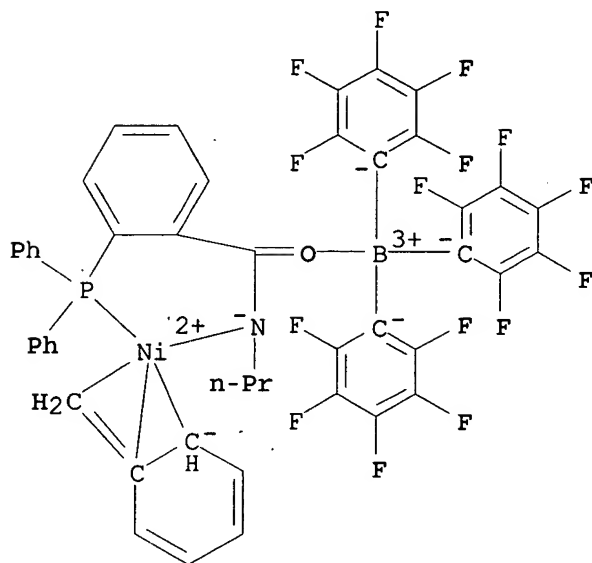
(preparation, crystal structure, and catalytic activity of (diphenylphosphinyl)benzamido nickel complexes)

RN 697288-94-1 HCAPLUS

CN Nickel, [μ -[N-(1,1-dimethylethyl)-2-(diphenylphosphino- κ P)benzamido- κ N: κ O]] (η 3-6-methylene-2,4-cyclohexadien-1-yl) [tris(pentafluorophenyl)boron] - (9CI) (CA INDEX NAME)

RN 697288-96-3 HCAPLUS

CN Nickel, [μ -[2-(diphenylphosphino- κ P)-N-propylbenzamido- κ N: κ O]] (η^3 -6-methylene-2,4-cyclohexadien-1-yl) [tris(pentafluorophenyl)boron]- (9CI) (CA INDEX NAME)



CC 29-13. (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 35, 67, 75

ST diphenylphosphinyl benzamide ligand prepn reaction nickel benzyl phosphine complex; nickel phosphinylbenzamido benzyl complex prepn structure reaction pentafluorophenyl borane; **zwitterionic** diphenylphosphinobenzamido benzyl nickel boron complex prepn structure catalyst; ethylene nickel diphenylphosphinobenzamido boron complex catalyzed polymn steric hindrance; butene polyethylene prepn; crystal structure diphenylphosphinylbenzamido benzyl nickel boron complex; mol structure diphenylphosphinylbenzamido benzyl nickel boron complex

IT Polymerization

Polymerization catalysts

Steric hindrance

Zwitterions

(preparation, crystal structure, and catalytic activity of (diphenylphosphinyl)benzamido nickel complexes)

IT 697288-93-0P 697288-97-4P

(crystal structure; preparation, crystal structure, and catalytic activity of (diphenylphosphinyl)benzamido nickel complexes)

IT 697289-02-4P 697289-03-5P 697751-12-5P

(crystal structure; preparation, crystal structure, and catalytic activity of (diphenylphosphinyl)benzamido nickel complexes)

IT 697288-91-8P 697288-92-9P

(mol. structure; preparation, crystal structure, and catalytic activity of (diphenylphosphinyl)benzamido nickel complexes)

IT 697288-94-1P 697288-96-3P

(preparation, crystal structure, and catalytic activity of (diphenylphosphinyl)benzamido nickel complexes)

REFERENCE COUNT:

60

THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 5 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:753398 HCAPLUS

DOCUMENT NUMBER: 139:381592

TITLE: [2-(Alkylideneamino)benzoato]nickel(II)
Complexes: Active Catalysts for Ethylene
PolymerizationAUTHOR(S): Shim, Chang Bo; Kim, Young Heui; Lee, Bun
Yeoul; Dong, Yongkwan; Yun, HoseopCORPORATE SOURCE: Department of Molecular Science and
Technology, Ajou University, Suwon, 442-749,
S. Korea

SOURCE: Organometallics (2003), 22(21), 4272-4280

CODEN: ORGND7; ISSN: 0276-7333

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:381592

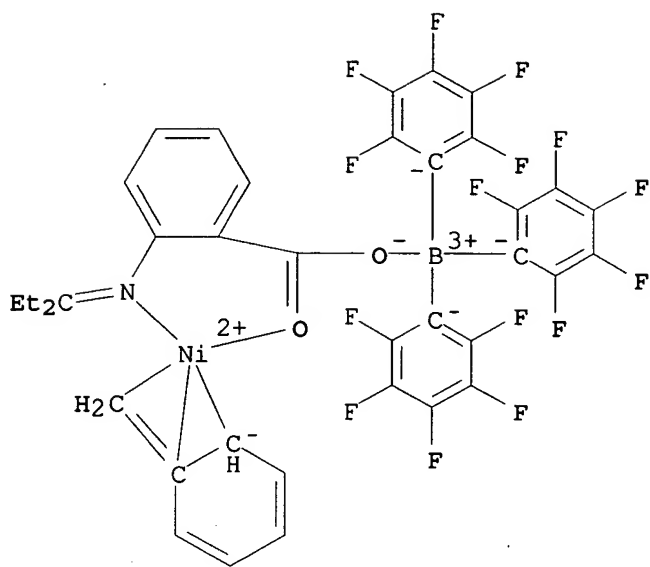
AB [RR'C:NC6H4C(O)O- κ 2N,O]Ni(η 3-CH2CMeCH2) (R, R' =
-(CH2)5-, 6; R = Et, R' = Et, 7; R = tBu, R' = H, 8) were prepared
by reaction of the corresponding K salts with [(η 3-
CH2CMeCH2)NiCl]₂ in MeCN. Addns. of 1 equiv of B(C6F5)₃ afford
the **zwitterionic** complexes [RR'C:NC6H4C{OB(C6F5)₃}O-
 κ 2N,O]Ni(η 3-CH2CMeCH2) (R, R' = -(CH2)5-, 9; R = Et, R'
= Et, 10; R = tBu, R' = H, 11), which give poly(ethylene) when
ethylene gas is added. This result is interesting in that the
corresponding 2-(diphenylphosphino)benzoato and
2-(diphenylamino)benzoato complexes give mainly butene. Reactions
of the K salts with Ni(η 3-CH2C6H5)Cl(PMe3) afford benzyl
complexes, [RR'C:NC6H4C(O)O- κ 2N,O]Ni(η 1-CH2C6H5)(PMe3)
(R, R' = -(CH2)5-, 12; R = Et, R' = Et, 13). Addns. of 2 equiv of
B(C6F5)₃ to 12 and 13 afford the **zwitterionic**
 η 3-benzyl complexes [RR'C:NC6H4C{OB(C6F5)₃}O-
 κ 2N,O]Ni(η 3-CH2C6H5) (R, R' = -(CH2)5-, 14; R = Et, R' =
Et, 15). Complex 14 is rather unstable, and a bis ligand complex,
[(CH2)5C:NC6H4C{OB(C6F5)₃}O- κ 2N,O]₂Ni (16), is formed during
recrystn. Complexes 14 and 15 are highly active to ethylene
polymerization, and activities reach 3000-4000 kg/((mol of Ni) h) at 75
psig pressure. Solid structures of 6, 9, 11, 15, and 16 were
determined by x-ray crystallog.

IT 623938-49-8P

(crystal structure; reaction of [(alkylideneamino)benzoato]nickel(II) complex with tris(pentafluorophenyl)borane to give
zwitterionic complexes as catalyst for ethylene
polymerization)

RN 623938-49-8 HCAPLUS

CN Nickel, [[2-[(1-ethylpropylidene)amino]benzoato-
 κ O]tris(pentafluorophenyl)borato(1-)-
 κ N, κ O'](η 3-6-methylene-2,4-cyclohexadien-1-yl)-
(9CI) (CA INDEX NAME)

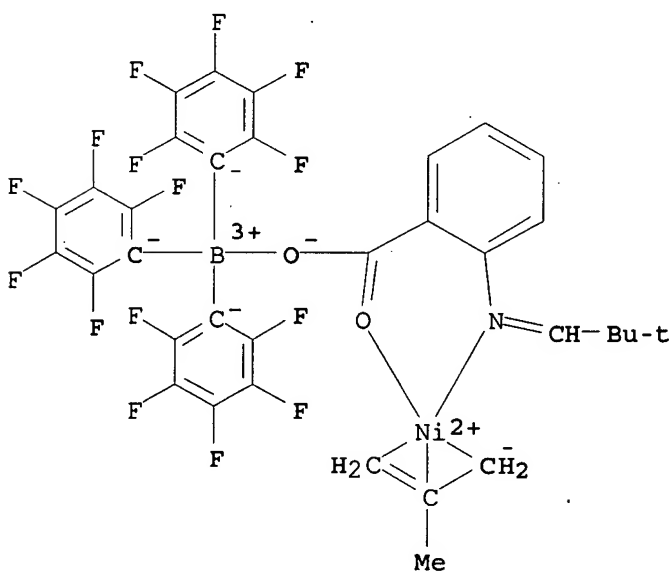


IT 623938-43-2P

(crystal structure; reaction of [(alkylideneamino)benzoato]nickel(II) complex with tris(pentafluorophenyl)borane to give zwitterionic complexes as catalyst for ethylene polymerization)

RN 623938-43-2 HCAPLUS

CN Nickel, [[2-[(Z)-(2,2-dimethylpropylidene)amino]benzoato- κ O]tris(pentafluorophenyl)borato(1-)- κ N, κ O'][(1,2,3- η)-2-methyl-2-propenyl]- (9CI) (CA INDEX NAME)



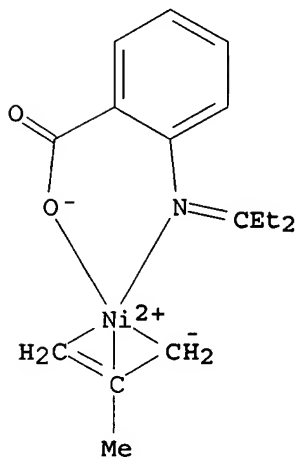
IT 623938-35-2P 623938-37-4P 623938-45-4P

(preparation and reaction of [(alkylideneamino)benzoato]nickel(II) complex with tris(pentafluorophenyl)borane to give

zwitterionic complexes as catalyst for ethylene
polymerization)

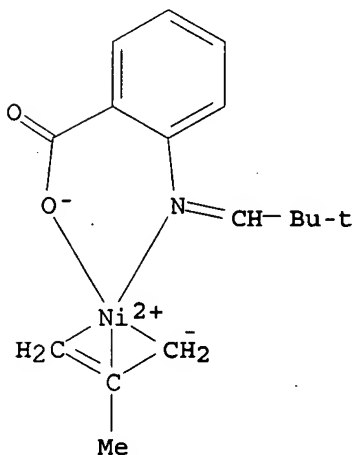
RN 623938-35-2 HCAPLUS

CN Nickel, [2-[(1-ethylpropylidene)amino- κ N]benzoato- κ O] [(1,2,3- η)-2-methyl-2-propenyl]- (9CI) (CA INDEX
NAME)



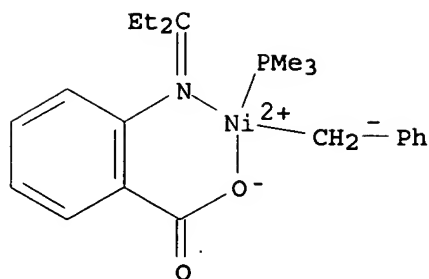
RN 623938-37-4 HCAPLUS

CN Nickel, [2-[(Z)-(2,2-dimethylpropylidene)amino- κ N]benzoato- κ O] [(1,2,3- η)-2-methyl-2-propenyl]- (9CI) (CA INDEX
NAME)



RN 623938-45-4 HCAPLUS

CN Nickel, [2-[(1-ethylpropylidene)amino- κ N]benzoato- κ O] (phenylmethyl) (trimethylphosphine)- (9CI) (CA INDEX
NAME)

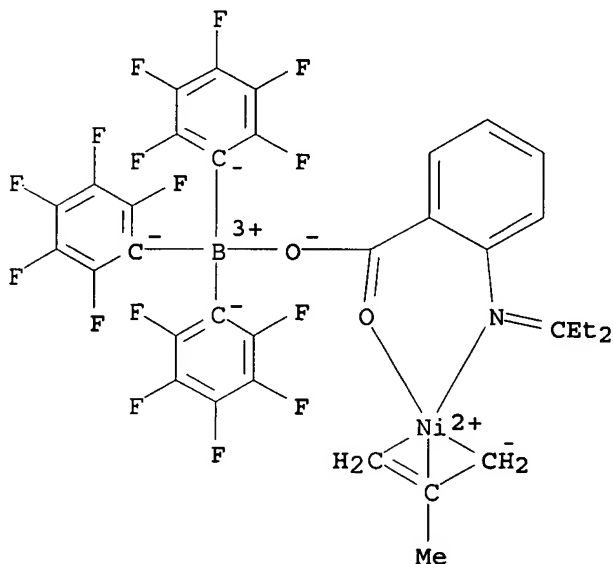


IT 623938-41-0P

(reaction of [(alkylideneamino)benzoato]nickel(II) complex with tris(pentafluorophenyl)borane to give **zwitterionic** complexes as catalyst for ethylene polymerization)

RN 623938-41-0 HCAPLUS

CN Nickel, [[2-[(1-ethylpropylidene)amino]benzoato- κ O]tris(pentafluorophenyl)borato(1-)- κ N, κ O'][(1,2,3- η)-2-methyl-2-propenyl]- (9CI) (CA INDEX NAME)



CC 29-13 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 75

ST mol crystal structure alkylideneamino benzoato nickel **zwitterionic** complex; crystal structure alkylideneamino benzoato nickel **zwitterionic** complex; alkylideneamino benzoato nickel **zwitterionic** complex prepn catalyst ethylene polymn

IT Crystal structure

Molecular structure

(of [(alkylideneamino)benzoato]nickel(II) complexes and their **zwitterionic** complexes)

IT Polymerization

Polymerization catalysts

Zwitterions

- (reaction of [(alkylideneamino)benzoato]nickel(II) complexes with tris(pentafluorophenyl)borane to give **zwitterionic** complexes as catalyst for ethylene polymerization)
- IT 74-85-1, Ethylene, reactions
([(alkylideneamino)benzoato]nickel(II) **zwitterionic** complex-catalyzed polymerization of ethylene)
- IT 623938-33-0P
(crystal structure; preparation and reaction of [(alkylideneamino)benzoato]nickel(II) complex with tris(pentafluorophenyl)borane to give **zwitterionic** complexes as catalyst for ethylene polymerization)
- IT 623938-49-8P
(crystal structure; reaction of [(alkylideneamino)benzoato]nickel(II) complex with tris(pentafluorophenyl)borane to give **zwitterionic** complexes as catalyst for ethylene polymerization)
- IT 623938-39-6P 623938-43-2P 623938-52-3P
(crystal structure; reaction of [(alkylideneamino)benzoato]nickel(II) complex with tris(pentafluorophenyl)borane to give **zwitterionic** complexes as catalyst for ethylene polymerization)
- IT 623938-51-2P
(mol. structure; reaction of [(alkylideneamino)benzoato]nickel(II) complex with tris(pentafluorophenyl)borane to give **zwitterionic** complexes as catalyst for ethylene polymerization)
- IT 96-22-0, 3-Pentanone
(of [(alkylideneamino)benzoato]nickel(II) complexes and their **zwitterionic** complexes)
- IT 9002-88-4P, Polyethylene
(of [(alkylideneamino)benzoato]nickel(II) complexes and their **zwitterionic** complexes)
- IT 623938-35-2P 623938-37-4P 623938-44-3P
623938-45-4P
(preparation and reaction of [(alkylideneamino)benzoato]nickel(II) complex with tris(pentafluorophenyl)borane to give **zwitterionic** complexes as catalyst for ethylene polymerization)
- IT 623938-47-6P
(reaction of [(alkylideneamino)benzoato]nickel(II) complex with tris(pentafluorophenyl)borane to give **zwitterionic** complexes as catalyst for ethylene polymerization)
- IT 623938-41-0P
(reaction of [(alkylideneamino)benzoato]nickel(II) complex with tris(pentafluorophenyl)borane to give **zwitterionic** complexes as catalyst for ethylene polymerization)
- IT 1109-15-5, Tris(pentafluorophenyl)borane
(reaction of [(alkylideneamino)benzoato]nickel(II) complexes with tris(pentafluorophenyl)borane to give **zwitterionic** complexes as catalyst for ethylene polymerization)

REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 6 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:406085 HCAPLUS

DOCUMENT NUMBER: 139:197795

TITLE: N-(2-Benzoylphenyl)benzamido nickel(II) complexes and polymerization reactivity

AUTHOR(S): Shim, Chang Bo; Kim, Young Heui; Lee, Bun

CORPORATE SOURCE: Yeoul; Shin, Dong Mok; Chung, Young Keun
Department of Molecular Science and
Technology, Ajou University, Suwon, 442-749,
S. Korea

SOURCE: Journal of Organometallic Chemistry (2003),
675(1-2), 72-76
CODEN: JORCAI; ISSN: 0022-328X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

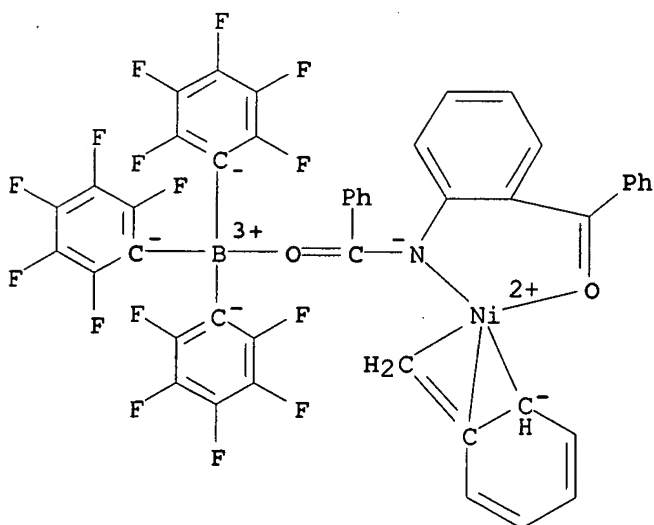
LANGUAGE: English

AB [N-(2-Benzoylphenyl)benzamido- κ^2 N,O] (η^1 -benzyl) (trimethylphosphine)Ni(II) (3) was prepared by the reaction of potassium N-(2-benzoylphenyl)benzamide and Ni(η^3 -CH₂C₆H₅)Cl(PMe₃). When 3 is treated with one equivalent of B(C₆F₅)₃, one obtains a zwitterionic complex, [PhC(O)-C₆H₄-N:C(Ph)OB(C₆F₅)₃- κ^2 N,O]Ni(η^1 -CH₂C₆H₅)(PMe₃) (4). When two equivalent of B(C₆F₅)₃ is added, PMe₃ is abstracted to give a η^3 -benzyl zwitterionic complex, [PhC(O)-C₆H₄-N:C(Ph)OB(C₆F₅)₃- κ^2 N,O]Ni(η^3 -CH₂C₆H₅) (5). Solid structures of 4 and 5 were determined by X-ray crystallog. When ethylene was added to 5, low mol. weight polyethylene was obtained.

IT 585542-21-8P
(crystal structure of; preparation and reactivity of N-(2-Benzoylphenyl)benzamido nickel(II) complexes in polymerization of ethylene)

RN 585542-21-8 HCAPLUS

CN Nickel, [μ -[N-[2-(benzoyl- κ O)phenyl]benzamido- κ^2 N: κ O]] (η^3 -6-methylene-2,4-cyclohexadien-1-yl) [tris(pentafluorophenyl)boron]-, stereoisomer (9CI) (CA INDEX NAME)



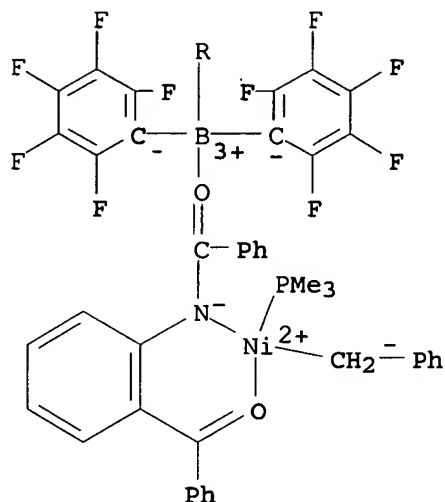
IT 585542-20-7P
(crystal structure of; preparation and reactivity of N-(2-Benzoylphenyl)benzamido nickel(II) complexes in polymerization of ethylene)

RN 585542-20-7 HCAPLUS

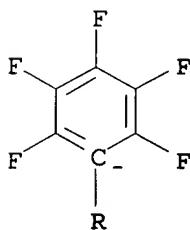
CN Nickel, [μ -[N-[2-(benzoyl- κ O)phenyl]benzamido- κ^2 N: κ O]] (phenylmethyl) (trimethylphosphine) [tris(pentafl

uorophenyl)boron] - (9CI) (CA INDEX NAME)

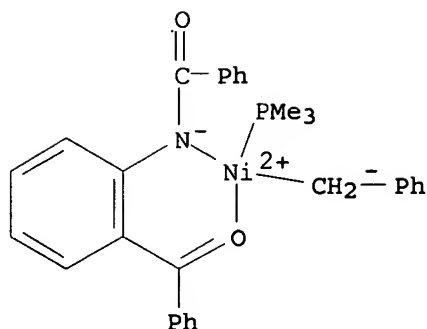
PAGE 1-A



PAGE 2-A



IT 585542-19-4P
 (preparation and reactivity of N-(2-Benzoylphenyl)benzamido
 nickel(II) complexes in polymerization of ethylene)
 RN 585542-19-4 HCAPLUS
 CN Nickel, [N-[2-(benzoyl-κO)phenyl]benzamido-
 κN] (phenylmethyl) (trimethylphosphine) - (9CI) (CA INDEX
 NAME)



CC 35-3 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 29, 75

IT 585542-21-8P

(crystal structure of; preparation and reactivity of N-(2-Benzoylphenyl)benzamido nickel(II) complexes in polymerization of ethylene)

IT 585542-20-7P

(crystal structure of; preparation and reactivity of N-(2-Benzoylphenyl)benzamido nickel(II) complexes in polymerization of ethylene)

IT 585542-19-4P

(preparation and reactivity of N-(2-Benzoylphenyl)benzamido nickel(II) complexes in polymerization of ethylene)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 7 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:326586 HCAPLUS

DOCUMENT NUMBER: 139:69362

TITLE: Organometallic Complexes Containing a Co-N-C Three-Membered Ring: Factors Affecting the Dynamic of the Ring Closure

AUTHOR(S): Dreos, Renata; Felluga, Alessandro; Nardin, Giorgio; Randaccio, Lucio; Tauzher, Giovanni
CORPORATE SOURCE: Dipartimento di Scienze Chimiche, Universita di Trieste, Trieste, 34127, Italy

SOURCE: Organometallics (2003), 22(12), 2486-2491
CODEN: ORGND7; ISSN: 0276-7333

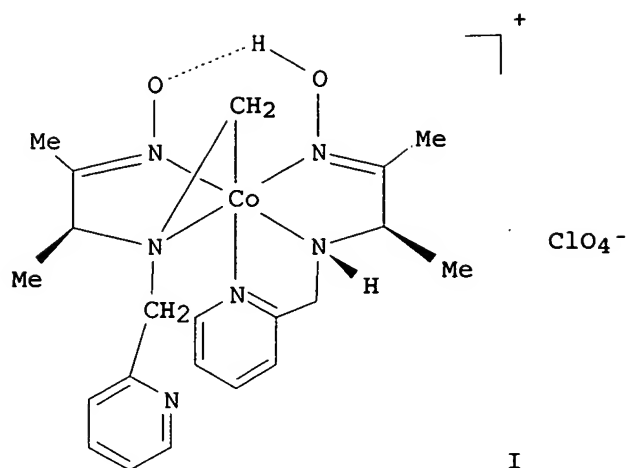
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:69362

GI



AB Treatment of $[\text{ClCH}_2\text{CoIII}(\text{L1NH-py})(\text{HL1NH-py})]\text{ClO}_4$, where HL1NH-py is the tridentate 2-((2-pyridylmethyl)amino)-3-butanone oxime and L1NH-py- its conjugated base, with diluted NaOH, afforded $[\text{CH}_2\text{CoIII}(\text{L1NH-py})(\text{HL1N-py})]\text{ClO}_4$ (I), containing a three-membered metallacycle by a pathway involving the intramol. nucleophilic addition of an equatorial N donor to the axial C. The x-ray anal. revealed a highly distorted structure with the distortion concentrated in the Co-C bond. The kinetics of formation of this complex and of the analogous complexes (previously synthesized), containing the 2-((2-(2-pyridyl)ethyl)amino)-3-butanone oxime ligand (HLNH-py), were studied. These studies revealed that the intramol. process forming the metallacycle is quite rapid, whereas the C atom bonded to Co is inert toward nucleophilic intermol. attack. The rapidity of the reaction was ascribed to a favorable entropy contribution and to the proximity effect imposed by the relatively rigid framework of the mol., which holds together the reactive centers (C and N atoms) within a critical distance.

IT 548739-91-9P

(base catalyzed ring closure; kinetic thermodyn. and other factors affecting intramol. ring closure leading to formation of 3-membered Co-N-C ring)

RN 548739-91-9 HCAPLUS

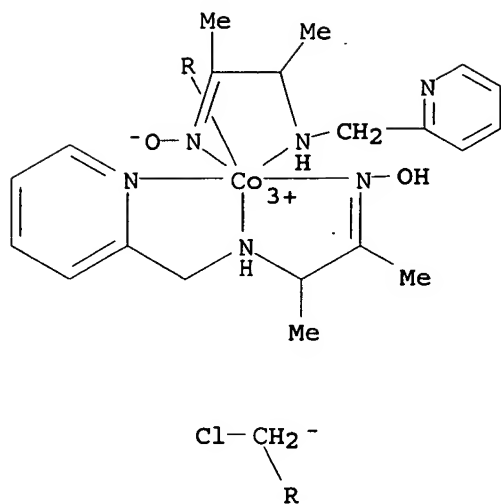
CN Cobalt(1+), rel-(chloromethyl)[(3S)-3-[(R)-(2-pyridinylmethyl)amino-κN]-2-butanone oximato-κN][(3R)-3-[(S)-[(2-pyridinyl-κN)methyl]amino-κN]-2-butanone oxime-κN]-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 548739-90-8

CMF C21 H31 Cl Co N6 O2

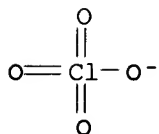
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



IT 548739-93-1P

(crystal structure; kinetic thermodyn. and other factors affecting intramol. ring closure leading to formation of 3-membered Co-N-C ring)

RN 548739-93-1 HCAPLUS

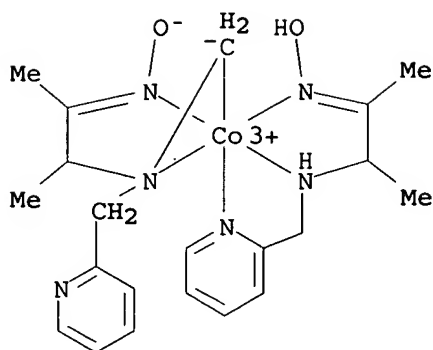
CN Cobalt(1+), rel-[[(R) - [(1S) - 2-(hydroxylatoimino-κN) - 1-methylpropyl] (2-pyridinylmethyl) amino-κN]methyl-κC] [(3S) - 3-[(R) - [(2-pyridinyl-κN)methyl] amino-κN] - 2-butanone oxime-κN] -, (OC-6-45) -, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 548739-92-0

CMF C21 H30 Co N6 O2

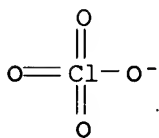
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4

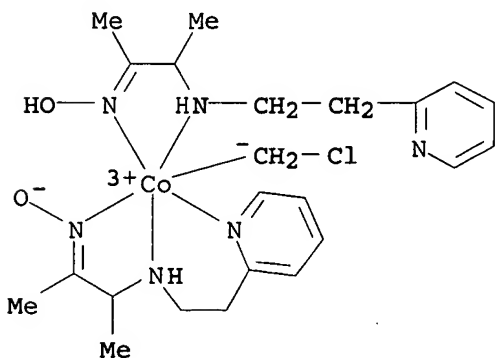


IT 329969-39-3 377734-71-9 377734-80-0

(kinetic thermodyn. and other factors affecting intramol. ring closure leading to formation of 3-membered Co-N-C ring)

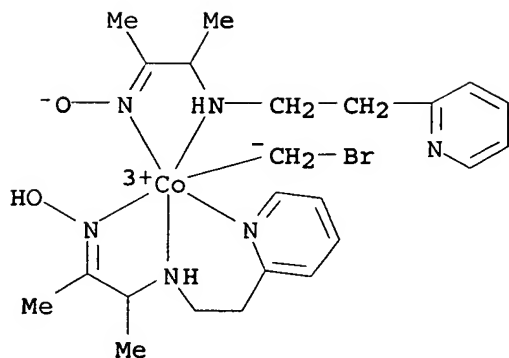
RN 329969-39-3 HCAPLUS

CN Cobalt(1+), rel-(chloromethyl) [(3R)-3-[(S)-[2-(2-pyridinyl-κN)ethyl]amino-κN]-2-butanone oximate-κN] [(3R)-3-[(S)-[2-(2-pyridinyl)ethyl]amino-κN]-2-butanone oxime-κN]-, (OC-6-54)- (9CI) (CA INDEX NAME)



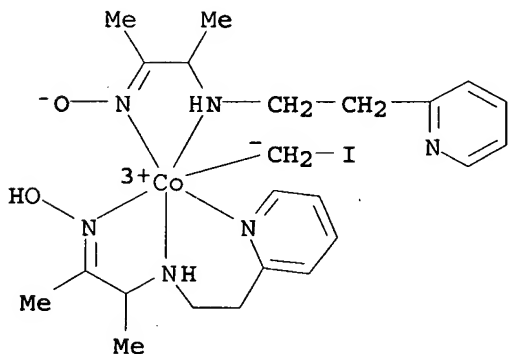
RN 377734-71-9 HCAPLUS

CN Cobalt(1+), rel-(bromomethyl) [(3R)-3-[(S)-[2-(2-pyridinyl)ethyl]amino-κN]-2-butanone oximate-κN] [(3R)-3-[(S)-[2-(2-pyridinyl-κN)ethyl]amino-κN]-2-butanone oxime-κN]-, (OC-6-54)- (9CI) (CA INDEX NAME)



RN 377734-80-0 HCAPLUS

CN Cobalt(1+), rel-(iodomethyl)[(3R)-3-[(S)-[2-(2-pyridinyl)ethyl]amino-κN]-2-butanone oximate-κN][(3R)-3-[(S)-[2-(2-pyridinyl-κN)ethyl]amino-κN]-2-butanone oxime-κN]-, stereoisomer (9CI) (CA INDEX NAME)



CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22, 75

IT 548739-91-9P

(base catalyzed ring closure; kinetic thermodyn. and other factors affecting intramol. ring closure leading to formation of 3-membered Co-N-C ring)

IT 548739-93-1P

(crystal structure; kinetic thermodyn. and other factors affecting intramol. ring closure leading to formation of 3-membered Co-N-C ring)

IT 329969-39-3 377734-71-9 377734-80-0

(kinetic thermodyn. and other factors affecting intramol. ring closure leading to formation of 3-membered Co-N-C ring)

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 8 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:298267 HCAPLUS

DOCUMENT NUMBER: 139:36626

TITLE: A Catalytically Active, Charge-Neutral Rh(I)

Zwitterion Featuring a P,N-Substituted "Naked" Indenide Ligand

AUTHOR(S): Stradiotto, Mark; Cipot, Judy; McDonald, Robert

CORPORATE SOURCE: Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, B3H 4J3, Can.

SOURCE: Journal of the American Chemical Society (2003), 125(19), 5618-5619
CODEN: JACSAT; ISSN: 0002-7863

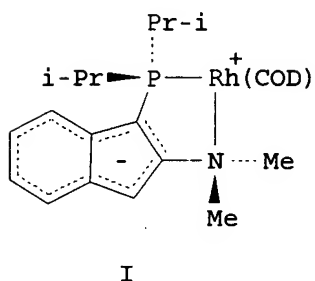
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:36626

GI



AB The synthesis and characterization of a new class of cationic and **zwitterionic** Rh(I) complexes, e.g. I, which feature multidentate ligands comprised of donor-functionalized indene or indenide units, are reported. This unusual new ligation strategy provides access to the first charge-neutral [κ^2 -P,N]Rh(I) **zwitterion**, a complex that functions as a catalyst for the C-H/Si-H dehydrogenative coupling of styrene and triethylsilane. Lithiation of 2-dimethylaminoindene followed by sequential phosphination with $i\text{Pr}_2\text{P}\text{Cl}$, complexation with $[(\text{COD})\text{RhCl}]_2$, chloride abstraction with AgBF_4 , and deprotonation with BuLi gave title complex I which was used as hydrosilylation catalyst for styrene with Et_3SiH . The crystal structure of I and intermediates were determined

IT **540492-55-5P**
(crystal structure; preparation, crystal structure, and hydrosilylation catalytic activity of neutral and cationic rhodium naked amino(phosphino)indenide ligand complex)

RN 540492-55-5 HCAPLUS

CN Rhodium, [1-[bis(1-methylethyl)phosphoranylidene- κP]-N,N-dimethyl-1H-inden-2-aminato- κN][(1,2,5,6- η)-1,5-cyclooctadiene]- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT **540492-60-2P**
(crystal structure; preparation, crystal structure, and hydrosilylation catalytic activity of neutral and cationic rhodium naked amino(phosphino)indenide ligand complex)

RN 540492-60-2 HCAPLUS

CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][3-

[bis(1-methylethyl)phosphino- κ P]-N,N-dimethyl-1H-inden-2-amine- κ N]-, tetrafluoroborate(1-), compd. with tetrahydrofuran (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 109-99-9

CMF C4 H8 O



CM 2

CRN 540492-58-8

CMF C24 H34 N P Rh . B F4

CM 3

CRN 540492-57-7

CMF C24 H34 N P Rh

CCI CCS

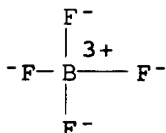
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 4

CRN 14874-70-5

CMF B F4

CCI CCS



IT 540492-58-8P

(mol. structure; preparation, crystal structure, and hydrosilylation catalytic activity of neutral and cationic rhodium naked amino(phosphino)indenide ligand complex)

RN 540492-58-8 HCAPLUS

CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene] [3-[bis(1-methylethyl)phosphino- κ P]-N,N-dimethyl-1H-inden-2-amine- κ N]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 540492-57-7

CMF C24 H34 N P Rh

CCI CCS

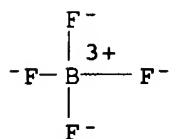
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 14874-70-5

CMF B F4

CCI CCS



IT 540492-54-4P

(preparation, crystal structure, and hydrosilylation catalytic activity of neutral and cationic rhodium naked amino(phosphino)indenide ligand complex)

RN 540492-54-4 HCAPLUS

CN Rhodium(1+), [3-[bis(1-methylethyl)phosphino-κP]-N,N-dimethyl-1H-inden-2-amine-κN] [(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 540492-53-3

CMF C25 H38 N P Rh

CCI CCS

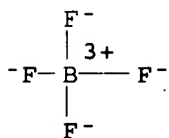
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 14874-70-5

CMF B F4

CCI CCS



CC 29-13 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 25, 75

ST charge neutral rhodium zwitterion phosphorus nitrogen indenide complex prepn; phosphino amino indenide rhodium complex prepn hydrosilylation catalyst; dehydrogenative coupling catalyst aminophosphino rhodium complex styrene triethylsilane; crystal mol structure aminophosphino indenide rhodium neutral cationic complex

IT 540492-55-5P

(crystal structure; preparation, crystal structure, and hydrosilylation catalytic activity of neutral and cationic rhodium naked amino(phosphino)indenide ligand complex)

IT 540492-59-9P 540492-60-2P

(crystal structure; preparation, crystal structure, and hydrosilylation catalytic activity of neutral and cationic rhodium naked amino(phosphino)indenide ligand complex)

IT 540492-58-8P
 (mol. structure; preparation, crystal structure, and hydrosilylation catalytic activity of neutral and cationic rhodium naked amino(phosphino)indenide ligand complex)

IT 540492-54-4P
 (preparation, crystal structure, and hydrosilylation catalytic activity of neutral and cationic rhodium naked amino(phosphino)indenide ligand complex)

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 9 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:502152 HCAPLUS

DOCUMENT NUMBER: 137:253851

TITLE: Structure, Stability, and Lability of Copper(II) Complexes with Triglycine

AUTHOR(S): Ilakin, V. S.; Shtyrlin, V. G.; Zakharov, A. V.; Kon'kin, A. L.

CORPORATE SOURCE: Kazan State University, Kazan, Russia

SOURCE: Russian Journal of General Chemistry (Translation of Zhurnal Obshchei Khimii) (2002), 72(3), 349-357

CODEN: RJGCEK; ISSN: 1070-3632

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal

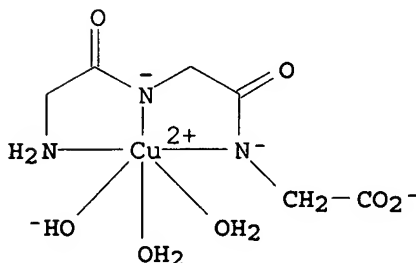
LANGUAGE: English

AB Equilibrium consts. of complex formation, rate consts. of chemical exchange reactions, and characteristics of electronic absorption spectra for species detected in aqueous solution of copper(II) with triglycine were determined, and conclusions on the structure of the complexes were made. A possibility of H-bond formation between the ammonium group of the zwitter-ionic form of the ligand and the second peptide oxygen in the anionic form of an adjacent ligand was shown. Kinetics and mechanisms of ligand and proton exchanges in solns. of copper(II) bistriptide complexes with the ligand containing a deprotonated peptide nitrogen atom were studied. A new mechanism was proposed for hydroxide-catalyzed substitution reactions in copper(II) complexes with tripeptides.

IT 460722-73-0 460722-78-5
 (structure, stability, and lability of copper(II) complexes with triglycine)

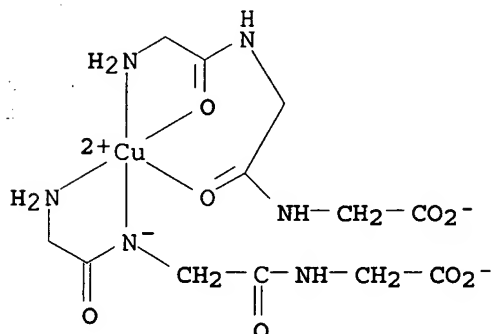
RN 460722-73-0 HCAPLUS

CN Cuprate(2-), diaqua[glycyl-κN-glycyl-κN-glycinato(3-)-κN]hydroxy-, (OC-6-14)- (9CI) (CA INDEX NAME)



RN 460722-78-5 HCAPLUS

CN Cuprate(1-), (glycyl-κN,κO-glycyl-κO-glycinato)[glycyl-κN-glycyl-κN-glycinato(2-)]- (9CI)
(CA INDEX NAME)



CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)

Section cross-reference(s): 34, 78

IT Complexation

Equilibrium constant

Exchange reaction kinetics

Formation constant

Hydrogen bond

Molecular structure

Stability

Zwitterions

(structure, stability, and lability of copper(II) complexes with triglycine)

IT 556-33-2D, Triglycine, copper complexes 7440-50-8D, Copper, triglycine complexes 122423-97-6 460722-66-1 460722-68-3 460722-70-7 460722-73-0 460722-78-5

(structure, stability, and lability of copper(II) complexes with triglycine)

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 10 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:301220 HCAPLUS

DOCUMENT NUMBER: 137:33579

TITLE: Catalytic Copolymerization of CO and Ethylene with a Charge Neutral Palladium(II) Zwitterion

AUTHOR(S): Lu, Connie C.; Peters, Jonas C.

CORPORATE SOURCE: Division of Chemistry and Chemical Engineering, Arnold and Mabel Beckman Laboratories of Chemical Synthesis, California Institute of Technology, Pasadena, CA, 91125, USA

SOURCE: Journal of the American Chemical Society (2002), 124(19), 5272-5273
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The synthesis of a zwitterionic Pd(II) complex supported

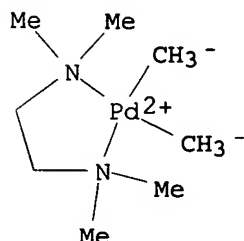
by an anionic bis(phosphino)borate ligand, $\text{Ph}_2\text{B}(\text{CH}_2\text{PPh}_2)_2$ (abbreviated as $[\text{Ph}_2\text{BP}_2]$), is reported. The new complex, $[\text{Ph}_2\text{BP}_2]\text{PdMe}(\text{THF})$, is active for CO and ethylene copolymer. The copolymer activity and polyketone mol. weight for the neutral, **zwitterionic** system are compared with those for the cationic systems $[\text{R}_2\text{E}(\text{CH}_2\text{PPh}_2)_2\text{PdMe}(\text{THF})][\text{B}(\text{C}_6\text{F}_5)_4]$ where $\text{ER}_2 = \text{SiPh}_2$ and CH_2 . Surprisingly, the more electron rich **zwitterionic** system is a catalyst of activity comparable to that of the more conventional cationic systems.

IT 113822-11-0

(catalyst synthesis; mechanism of catalytic copolymer. of CO and ethylene with **zwitterionic** Pd(II) complex supported by an anionic bis(phosphino)borate ligand)

RN 113822-11-0 HCAPLUS

CN Palladium, dimethyl(N,N,N',N'-tetramethyl-1,2-ethanediamine- $\kappa\text{N},\kappa\text{N}'$)-, (SP-4-2)- (9CI) (CA INDEX NAME)



CC 35-3 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 29, 75

ST palladium phosphinoborate **zwitterion** catalyst ethylene polymer carbon monoxide

IT Polymerization catalysts

(mechanism of catalytic copolymer. of CO and ethylene with **zwitterionic** Pd(II) complex supported by an anionic bis(phosphino)borate ligand)

IT 437711-99-4

(CO insertion complex; mechanism of catalytic copolymer. of CO and ethylene with **zwitterionic** Pd(II) complex supported by an anionic bis(phosphino)borate ligand)

IT 113822-11-0 350480-00-1

(catalyst synthesis; mechanism of catalytic copolymer. of CO and ethylene with **zwitterionic** Pd(II) complex supported by an anionic bis(phosphino)borate ligand)

IT 437712-00-0P

(crystal structure, catalyst dimerization product; mechanism of catalytic copolymer. of CO and ethylene with **zwitterionic** Pd(II) complex supported by an anionic bis(phosphino)borate ligand)

IT 437711-98-3

(ethylene insertion product; mechanism of catalytic copolymer. of CO and ethylene with **zwitterionic** Pd(II) complex supported by an anionic bis(phosphino)borate ligand)

IT 437711-96-1

(mechanism of catalytic copolymer. of CO and ethylene with **zwitterionic** Pd(II) complex supported by an anionic bis(phosphino)borate ligand)

IT 25052-62-4P, Carbon monoxide-ethylene copolymer

(mechanism of catalytic copolymer. of CO and ethylene with

zwitterionic Pd(II) complex supported by an anionic
bis(phosphino)borate ligand)

IT 437711-97-2P

(mol. structure, catalyst dimerization product; mechanism of
catalytic copolymn. of CO and ethylene with

zwitterionic Pd(II) complex supported by an anionic
bis(phosphino)borate ligand)

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L28 ANSWER 11 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:886261 HCAPLUS

DOCUMENT NUMBER: 136:20366

TITLE: Polymerization of olefins catalyzed by
transition metal complexes of selected
iminocarboxylate and iminoamido ligands
INVENTOR(S): Wang, Lin; Johnson, Lynda K.; Ionkin, Alex S.
PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
SOURCE: PCT Int. Appl., 58 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 5

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001092348	A2	20011206	WO 2001-US17636	2001 0531
WO 2001092348	A3	20020725		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2408663	AA	20011206	CA 2001-2408663	2001 0531
US 2002028741	A1	20020307	US 2001-871100	2001 0531
US 6506861	B2	20030114		
EP 1290043	A2	20030312	EP 2001-948254	2001 0531
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001011338	A	20030617	BR 2001-11338	2001 0531
JP 2003535107	T2	20031125	JP 2002-500959	

US 2003130449	A1	20030710	US 2002-272765	2001 0531
US 2003130453	A1	20030710	US 2002-273049	2002 1017
US 2005043496	A1	20050224	US 2004-943199	2002 1017
PRIORITY APPLN. INFO.:			US 2000-208087P	P 2004 0916
			US 2000-211601P	P 2000 0531
			US 2000-214036P	P 2000 0615
			US 2001-871009	A3 2000 0623
			US 2001-871100	A3 2001 0530
			WO 2001-US17636	W 2001 0531

OTHER SOURCE(S): MARPAT 136:20366

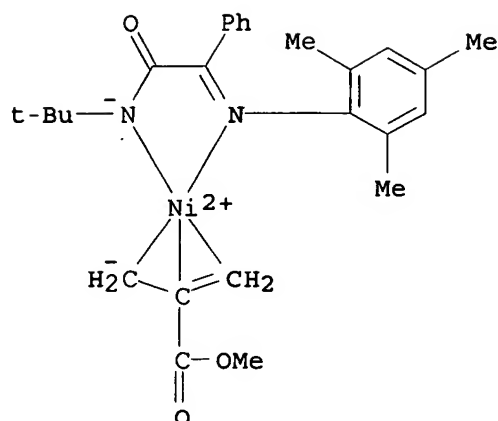
AB Olefins are polymerized by novel transition metal complexes of selected iminocarboxylate and iminoamido ligands, sometimes in the presence of cocatalysts such as alkylaluminum compds. or neutral Lewis acids. Olefins which may be (co)polymerized include ethylene, α -olefins, and olefins containing polar groups such as olefinic esters for example acrylate esters. Also described are certain "Zwitterionic" transition metal complexes as polymerization catalysts for making polar copolymers. The resulting polymers are useful as thermoplastics and elastomers.

IT 378793-67-0P

(polymerization of olefins catalyzed by transition metal complexes of selected iminocarboxylate and iminoamido ligands)

RN 378793-67-0 HCAPLUS

CN Nickel, [N-(1,1-dimethylethyl)- α -[(2,4,6-trimethylphenyl)imino- κ N]benzeneacetamidato- κ N] [(1,2,3- η)-2-(methoxycarbonyl)-2-propenyl]- (9CI) (CA INDEX NAME)



IC ICM C08F010-00

CC 35-4 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 67

IT 378793-60-3P 378793-61-4P 378793-62-5P 378793-63-6P

378793-64-7P 378793-65-8P 378793-66-9P 378793-67-0P

378793-68-1P 378793-69-2P

(polymerization of olefins catalyzed by transition metal complexes of selected iminocarboxylate and iminoamido ligands)

L28 ANSWER 12 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:659464 HCAPLUS

DOCUMENT NUMBER: 135:358007

TITLE: B(C₆F₅)₃ as C₆F₅ Transfer Agent in Zirconium Chemistry: Borole Sandwich and Borole-Bridged Triple-Decker Complexes

AUTHOR(S): Woodman, Timothy J.; Thornton-Pett, Mark; Hughes, David L.; Bochmann, Manfred

CORPORATE SOURCE: Wolfson Materials and Catalysis Centre School of Chemical Sciences, University of East Anglia, Norwich, NR4 7TJ, UK

SOURCE: Organometallics (2001), 20(19), 4080-4091

CODEN: ORGND7; ISSN: 0276-7333

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:358007

AB Treatment of Cp''Zr(C₆F₅)(OEt₂){η⁵-(3-RC₄H₃BC₆F₅)} (1H, R = H; 1Me, R = Me; Cp'' = 1,3-C₅H₃(SiMe₃)₂) in toluene with nitriles R'CN gives rise to the adducts Cp''Zr(C₆F₅)(NCR'){η⁵-(3-RC₄H₃BC₆F₅)} (2H, R = H, R' = Me; 3H, R = H, R' = t-Bu; 3Me, R = Me, R' = tBu) in high yields. The reaction of 1H and 1Me with a 4-fold excess of tert-Bu isocyanide in toluene at -20° leads to the formation of Cp''Zr(C₆F₅)(CNTBu)₂{η⁵-(3-RC₄H₃BC₆F₅)} (4H, R = H; 4Me, R = Me), while warming to room temperature results in the insertion of one mol. of isocyanide into the zirconium-C₆F₅ bond to give the η²-iminoacyl complexes Cp''Zr{η²-(C₆F₅CNTBu)}(CNTBu){η⁵-(3-RC₄H₃BC₆F₅)} (5H, R = H; 5Me, R = Me). The structures of 3H and 5H were confirmed by x-ray diffraction. The reaction of the diene complexes CpRZr(η³-crotyl)(η⁴-butadiene) (6a, CpR = C₅H₄SiMe₃; 6b, C₅H₄Me; 6c, Cp; 6d, Cp'') with B(C₆F₅)₃ in toluene solution at room temperature proceeds quant. with C-H activation, butene elimination, and

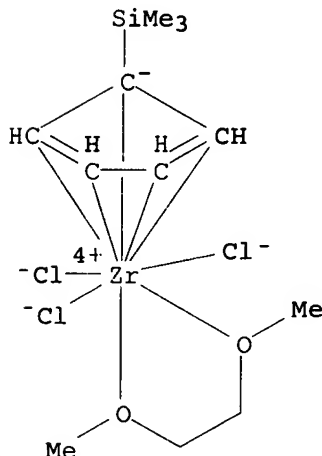
C6F5 transfer to generate $\text{CpRZr}(\text{C}_6\text{F}_5)\{\eta^4\text{-CH}_2\text{CHCHCHB}(\text{C}_6\text{F}_5)_2\}$ (7a-d). These boryldiene complexes are thermally unstable and smoothly rearrange to give the triple-decker complexes $\text{Zr}_2(\text{CpR})_2(\text{C}_6\text{F}_5)_2\{\mu\text{-}\eta^5\text{:}\eta^5\text{-C}_4\text{H}_4\text{BCH}_2\text{-}\eta^3\text{:}\kappa\text{F-CHCHCHB}(\text{C}_6\text{F}_5)_3\}$ (8a-d). The formation of these complexes involves the complete transfer of all three C6F5 substituents of one $\text{B}(\text{C}_6\text{F}_5)_3$ mol., as well as C-H activation and the loss of one C6F5 group as pentafluorobenzene. The triple-decker complexes feature a $\text{Zr}_2\text{C}_4\text{B}$ core, a zwitterionic structure, and an unusually strong Zr-F donor interaction. On activation with methylaluminoxane (MAO), 8a-d polymerize ethene.

IT 263751-13-9

(Grignard reaction with crotyl-magnesium chloride)

RN 263751-13-9 HCAPLUS

CN Zirconium, trichloro[1,2-di(methoxy- κ O)ethane] [(1,2,3,4,5- η)-1-(trimethylsilyl)-2,4-cyclopentadien-1-yl]- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 35, 75

IT 263751-13-9

(Grignard reaction with crotyl-magnesium chloride)

REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 13 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:113075 HCAPLUS

DOCUMENT NUMBER: 126:104178

TITLE: Synthesis, Structural Characterization, and Reactivity of Zirconium Complexes Containing Trimethylenemethane-Based Ligands

AUTHOR(S): Rodriguez, George; Bazan, Guillermo C.
CORPORATE SOURCE: Department of Chemistry, University of Rochester, Rochester, NY, 14627-0216, USA

SOURCE: Journal of the American Chemical Society (1997), 119(2), 343-352

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 126:104178

AB General synthetic routes to Zr metallocene-like complexes containing derivs. of the dianionic trimethylenemethane (TMM) ligand are presented. One approach consists of reacting the dilithium salts of TMM, tribenzylidenemethane (TBM), tert-butyltribenzylidenemethane (t-Bu-TBM), and dibenzylidenemethylenemethane (DBM) with either Cp^*ZrCl_3 or $\text{CpZrCl}_3(\text{DME})$. In the case of the small TMM fragment, the product is the zwitterionic $\text{Cp}^*(\text{TMM})\text{Zr}(\mu\text{-Cl})_2\text{Li}(\text{TMEDA})$ (1). Larger TMM derivs. give discrete salts such as $[\text{Cp}^*(\text{TBM})\text{ZrCl}_2][\text{Li}(\text{TMEDA})_2]$ (2), $[\text{Cp}(\text{TBM})\text{ZrCl}_2][\text{Li}(\text{TMEDA})_2]$ (3), $[\text{Cp}(\text{t-Bu-TBM})\text{ZrCl}_2][\text{Li}(\text{TMEDA})_2]$ (4), $[\text{Cp}^*(\text{t-Bu-TBM})\text{ZrCl}_2][\text{Li}(\text{TMEDA})_2]$ (5), and $[\text{Cp}^*(\text{exo-endo-DBM})\text{ZrCl}_2][\text{Li}(\text{TMEDA})_2]$ (6). The reaction of $\text{TBM}(\text{LiTMEDA})_2$ with $\text{Cp}^*\text{ZrCl}_2\text{CH}_2\text{Ph}$ affords $[\text{Cp}^*(\text{TBM})\text{ZrCl}(\text{CH}_2\text{Ph})][\text{Li}(\text{TMEDA})_2]$ (9); thus the retention of $\text{LiCl}(\text{TMEDA})_2$ by Zr is strong. Structural characterization of these complexes reveals crowded environments around the Zr, especially when both TBM and Cp^* are coordinated. It is also possible to take advantage of intramol. σ -bond metathesis reactions to convert coordinated allyl ligands to TMM-related fragments. For example, $[\text{Cp}^*(\text{TMM})\text{Zr}]_2(\mu\text{-CH}_2)$ (10) is derived from $\text{Cp}^*(\eta^3\text{-CH}_2\text{C}(\text{Me})\text{CH}_2)\text{ZrMe}_2$, and $\text{Cp}^*(\text{TBM})\text{ZrMe}(\text{THF})$ (12) is from $\text{Cp}^*(\text{PhCH}_2\text{C}(\text{CHPh})_2)\text{ZrMe}_2$ (11). Formation of the methylpropargyl complex $\text{Cp}^*(\text{TBM})\text{Zr}(\eta^3\text{-CH}_2\text{CCMe})$ (13) from $\text{Cp}^*(\text{TBM})\text{ZrMe}(\text{THF})$ and 2-butyne instead of a butenyl derivative is a consequence of steric constraints. Activation of 2-6 with methylaluminoxane affords homogeneous catalyst mixts. for polymerization of ethylene and 1,5-hexadiene and copolymn. of ethylene with 1-hexene. There is a strong correlation between catalyst precursor structure and reactivity. Polyethylene can also be prepared by pressurizing a vessel containing only $\text{Cp}^*(\text{TBM})\text{ZrMe}(\text{THF})$.

IT 185856-55-7P 185856-61-5P

(crystal structure, polymerization catalyst; preparation, structure, and reactivity of zirconium complexes containing trimethylenemethane-based ligands)

RN 185856-55-7 HCAPLUS

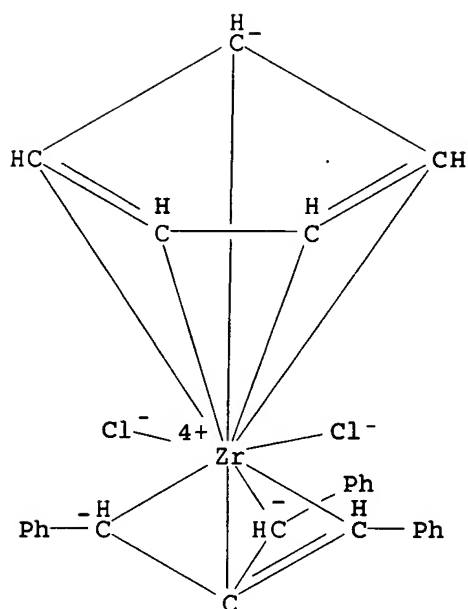
CN Lithium(1+), bis(N,N,N',N'-tetramethyl-1,2-ethanediamine- $\kappa\text{N},\kappa\text{N}'$)-, (T-4)-, stereoisomer of dichloro(η^5 -2,4-cyclopentadien-1-yl)[η^4 -1,3-diphenyl-2-(phenylmethylene)-1,3-propanediyl]zirconate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 185856-54-6

CMF C27 H23 Cl2 Zr

CCI CCS

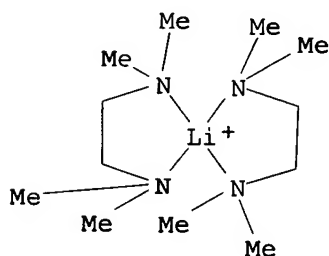


CM 2

CRN 57532-91-9

CMF C12 H32 Li N4

CCI CCS



RN 185856-61-5 HCAPLUS

CN Lithium(1+), bis(N,N,N',N'-tetramethyl-1,2-ethanediamine- κ N, κ N')-, (T-4)-, stereoisomer of dichloro(η 4-2-methylene-1,3-diphenyl-1,3-propanediyl) [(1,2,3,4,5- η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl] zirconate(1-) (9CI)
(CA INDEX NAME)

CM 1

CRN 185856-60-4

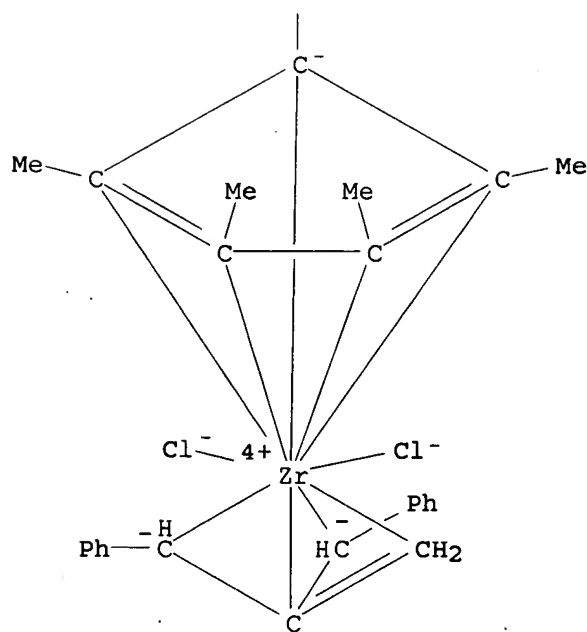
CMF C26 H29 Cl2 Zr

CCI CCS

PAGE 1-A

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PAGE 2-A

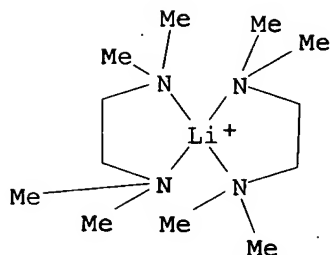


CM 2

CRN 57532-91-9

USHA SHRESTHA EIC 1700 REM 4B28

CMF C12 H32 Li N4
CCI CCS



IT 185856-63-7P
(crystal structure; preparation, structure, and reactivity of
zirconium complexes containing trimethylenemethane-based ligands)

RN 185856-63-7 HCAPLUS

CN Lithium(1+), bis(N,N,N',N'-tetramethyl-1,2-ethanediamine-
κN,κN')-, (T-4)-, stereoisomer of chloro[η4-1,3-
diphenyl-2-(phenylmethylene)-1,3-propanediyl] [(1,2,3,4,5-η)-
1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-
yl] (phenylmethyl)zirconate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 185856-62-6

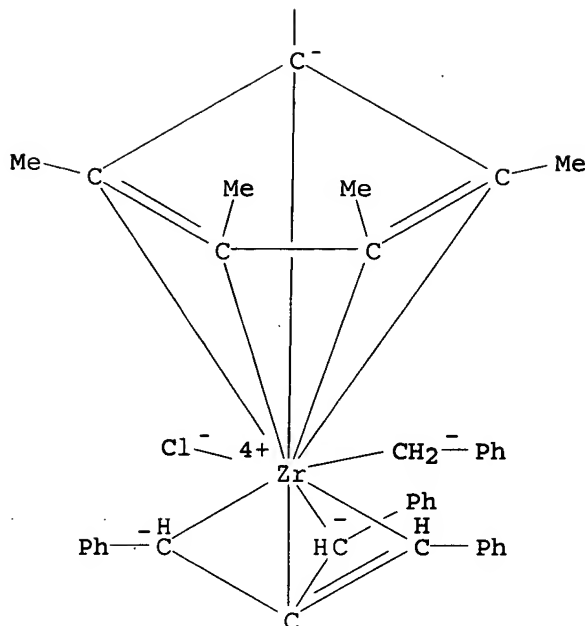
CMF C39 H40 Cl Zr

CCI CCS

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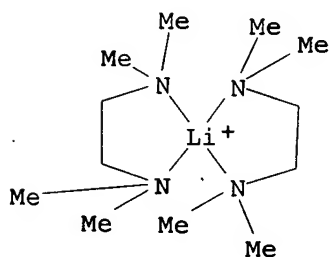


CM 2

CRN 57532-91-9

CMF C12 H32 Li N4

CCI CCS



IT 185856-57-9P 185856-59-1P

(mixture of isomers; preparation, structure, and reactivity of zirconium complexes containing trimethylenemethane-based ligands)

RN 185856-57-9 HCAPLUS

CN Lithium(1+), bis(N,N,N',N'-tetramethyl-1,2-ethanediamine- κ N, κ N')-, (T-4)-, dichloro(η 5-2,4-cyclopentadien-1-yl) [η 4-1-[4-(1,1-dimethylethyl)phenyl]-3-phenyl-2-(phenylmethylene)-1,3-propanediyl]zirconate(1-) (9CI) (CA INDEX NAME)

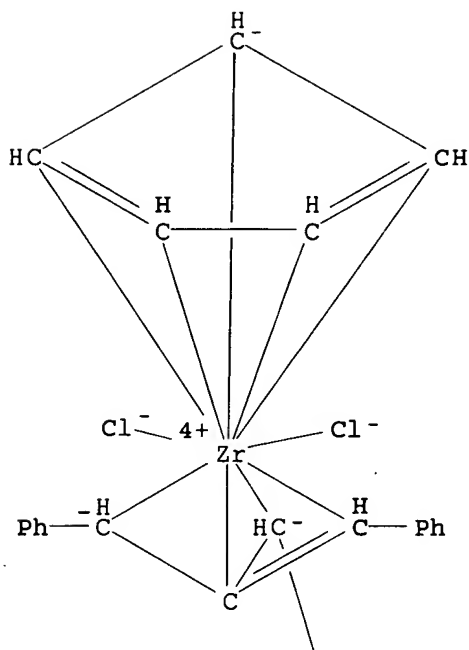
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CRN 185856-56-8

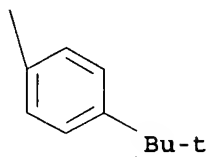
CMF C31 H31 Cl2 Zr

CCI CCS

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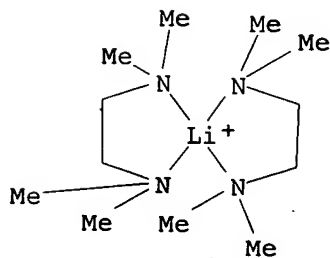


CM 2

CRN 57532-91-9

CMF C12 H32 Li N4

CCI CCS



RN 185856-59-1 HCAPLUS
CN Lithium(1+), bis(N,N,N',N'-tetramethyl-1,2-ethanediamine-
κN,κN')-, (T-4)-, dichloro[η4-1-[4-(1,1-
dimethylethyl)phenyl]-3-phenyl-2-(phenylmethylene)-1,3-
propanediyl][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-
cyclopentadien-1-yl]zirconate(1-) (9CI) (CA INDEX NAME)

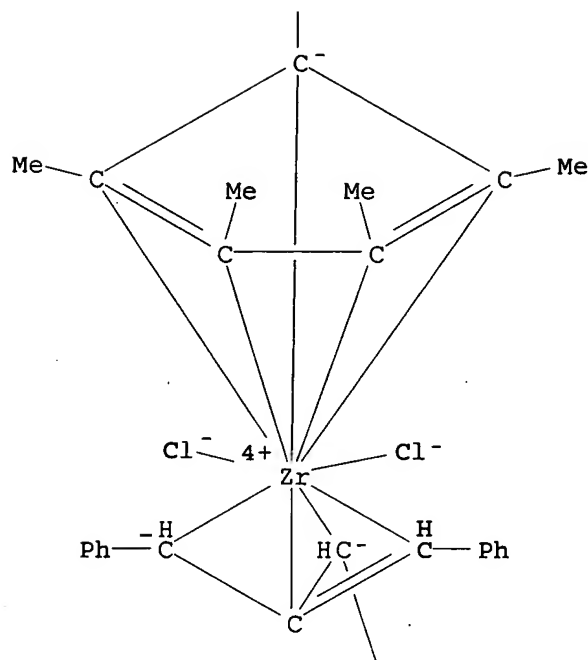
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CRN 185856-58-0
CMF C36 H41 Cl2 Zr
CCI CCS

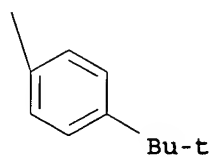
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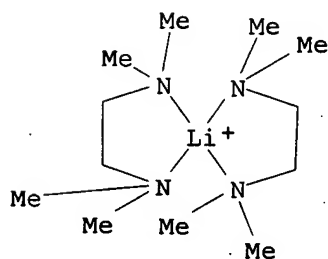


PAGE 3-A



CM 2

CRN 57532-91-9
 CMF C12 H32 Li N4
 CCI CCS



IT 154394-96-4

(polymerization catalyst; preparation, structure, and reactivity of zirconium complexes containing trimethylenemethane-based ligands)

RN 154394-96-4 HCAPLUS

CN Lithium(1+), (N,N,N',N'-tetramethyl-1,2-ethanediamine-
κN,κN')-, dichloro(η⁴-2-methylene-1,3-
propanediyl)[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-
cyclopentadien-1-yl]zirconate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 154394-95-3

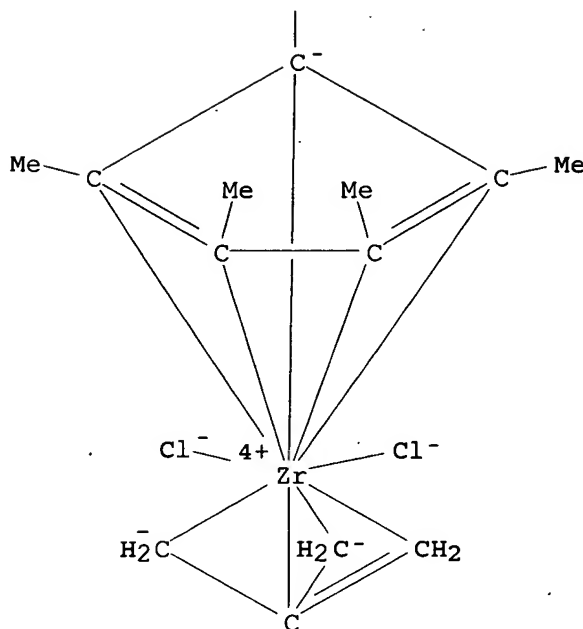
CMF C14 H21 Cl2 Zr

CCI CCS

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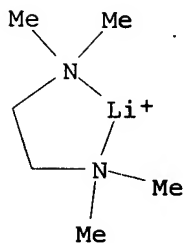
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CM 2

CRN 45651-70-5
 CMF C6 H16 Li N2
 CCI CCS



IT 154394-98-6P

(polymerization catalyst; preparation, structure, and reactivity of zirconium complexes containing trimethylenemethane-based ligands)

RN 154394-98-6 HCAPLUS

CN Lithium(1+), bis(N,N,N',N'-tetramethyl-1,2-ethanediamine- κ N, κ N')-, (T-4)-, dichloro[η 4-1,3-diphenyl-2-(phenylmethylene)-1,3-propanediyl][(1,2,3,4,5- η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]zirconate(1-) (9CI) (CA INDEX NAME)

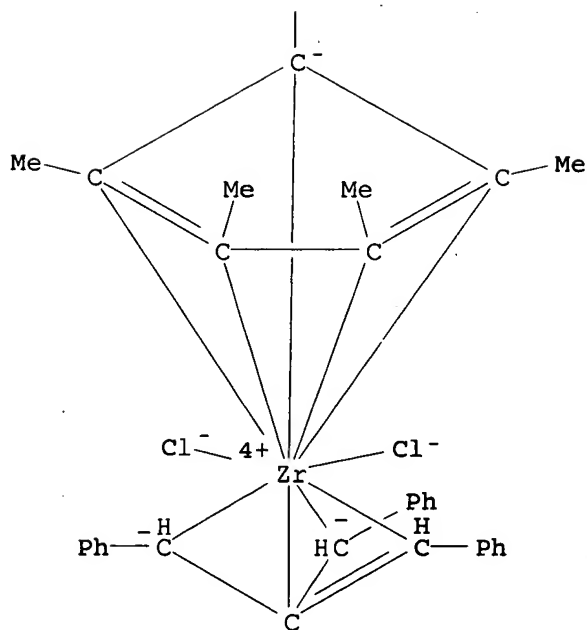
CM 1

CRN 154394-97-5
 CMF C32 H33 Cl2 Zr
 CCI CCS

PAGE 1-A

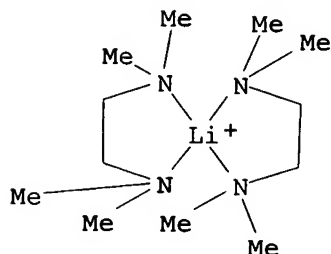


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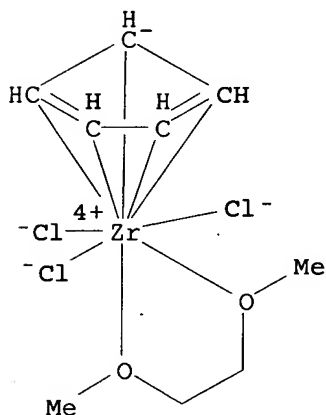
CRN 57532-91-9
 CMF C12 H32 Li N4
 CCI CCS



IT 79292-26-5
 (preparation, structure, and reactivity of zirconium complexes containing trimethylenemethane-based ligands)

RN 79292-26-5 HCAPLUS

CN Zirconium, trichloro(η^5 -2,4-cyclopentadien-1-yl) [1,2-di(methoxy- κ O)ethane]- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 35, 75

IT 185856-55-7P 185856-61-5P

(crystal structure, polymerization catalyst; preparation, structure, and reactivity of zirconium complexes containing trimethylenemethane-based ligands)

IT 185856-63-7P 185856-67-1P

(crystal structure; preparation, structure, and reactivity of zirconium complexes containing trimethylenemethane-based ligands)

IT 185856-57-9P 185856-59-1P

(mixture of isomers; preparation, structure, and reactivity of zirconium complexes containing trimethylenemethane-based ligands)

IT 154394-96-4

(polymerization catalyst; preparation, structure, and reactivity of zirconium complexes containing trimethylenemethane-based ligands)

IT 154394-98-6P

(polymerization catalyst; preparation, structure, and reactivity of zirconium complexes containing trimethylenemethane-based ligands)

IT 102-04-5, 1,3-Diphenylacetone 503-17-3, 2-Butyne 6921-34-2,

Benzylmagnesium chloride 33324-92-4, (2-Methylallyl)magnesium bromide 75181-07-6, Trichloro(pentamethylcyclopentadienyl)zirconium 79292-26-5 81476-67-7 81476-69-9 88227-25-2 92314-26-6 171508-05-7 850697-96-0
(preparation, structure, and reactivity of zirconium complexes containing trimethylenemethane-based ligands)

L28 ANSWER 14 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:796961 HCAPLUS

DOCUMENT NUMBER: 124:29369

TITLE: A study of chiral mixed ligand metal complexes and enzymes as **catalysts** in resolution of 1,1'-binaphthyl-2,2'-diol

AUTHOR(S): Thakkar, N. V.; Banerji, A. A.

CORPORATE SOURCE: Chem. Dep., Institute Science, Bombay, 400 032, India

SOURCE: Journal of the Indian Chemical Society (1995), 72(6), 421-3

CODEN: JICSAH; ISSN: 0019-4522

PUBLISHER: Indian Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

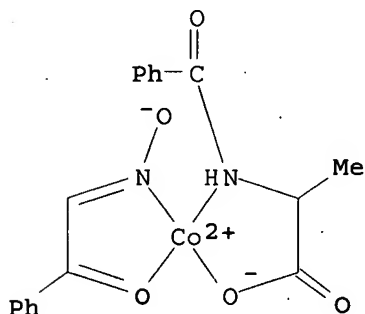
AB 1,1'-Binaphthyl-1,1'-diol diacetate was transesterified with methanol as a nucleophile as well as solvent in the presence of chiral mixed ligand metal complexes as well as lipases as **catalysts** to yield the diol of varying optical purity.

IT 171668-11-4 171668-12-5

(resolution of binaphthyldiol with chiral mixed ligand metal complexes and enzymes as **catalysts**)

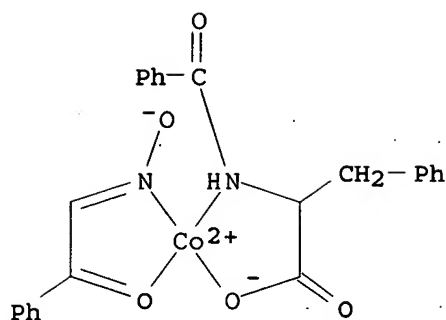
RN 171668-11-4 HCAPLUS

CN Cobalt, (N-benzoyl-L-alaninato-N,O1) (α -oxobenzeneacetaldehyde aldoximate)- (9CI) (CA INDEX NAME)



RN 171668-12-5 HCAPLUS

CN Cobalt, (N-benzoyl-L-phenylalaninato-N,O α) (α -oxobenzeneacetaldehyde aldoximate)- (9CI) (CA INDEX NAME)



- CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 Section cross-reference(s): 7
- ST resolu binaphthyldiol CMLM lipase; transesterification
catalysts enzymes CMLM
- IT Resolution
 (resolution of binaphthyldiol with chiral mixed ligand metal complexes and enzymes as **catalysts**)
- IT Transesterification **catalysts**
 (stereoselective, resolution of binaphthyldiol with chiral mixed ligand metal complexes and enzymes as **catalysts**)
- IT 18531-94-7P, [1,1'-Binaphthalene]-2,2'-diol, (R)- 18531-99-2P,
 [1,1'-Binaphthalene]-2,2'-diol, (S)-
 (resolution of binaphthyldiol with chiral mixed ligand metal complexes and enzymes as **catalysts**)
- IT 9001-62-1, Lipase 171668-07-8 171668-08-9 171668-09-0
 171668-10-3 171668-11-4 171668-12-5
 (resolution of binaphthyldiol with chiral mixed ligand metal complexes and enzymes as **catalysts**)
- IT 100569-82-2
 (resolution of binaphthyldiol with chiral mixed ligand metal complexes and enzymes as **catalysts**)

L28 ANSWER 15 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1993:409804 HCAPLUS

DOCUMENT NUMBER: 119:9804

TITLE: Metal chelates as colorants and

catalysts in epoxy resin compositions

INVENTOR(S): Boettcher, Axel; Hau, Reinhard; Doering,
 Manfred; Nitzsche, Klaus; Uhlig, Egon

PATENT ASSIGNEE(S): VEB Carl Zeiss, Germany

SOURCE: Ger. (East), 4 pp.

CODEN: GEXXA8

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

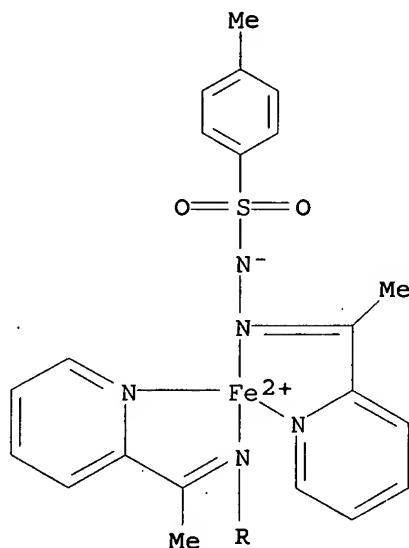
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 300735	A7	19920716	DD 1987-309796	1987 1130
PRIORITY APPLN. INFO.:				DD 1987-309796 1987

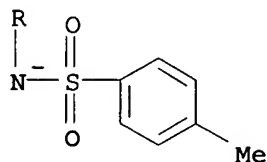
1130

- AB Complexes containing a metal ion such as Fe^{2+} , Fe^{3+} , or Co^{2+} and ligands such as 2-pyridyldiphenylcarbinol, N-allyl-N'-(p-tolylsulfonyl)thiourea, and 3-phenylsulfonamido-4,6-diphenylpyrimidine-2-thione are used as colorants and **catalysts** in the curing of mixts. of an epoxy resin and an amine hardener. The complex is selected to give the desired curing rate and product color. The cured compns. are transparent and useful in optoelectronics, etc.
- IT 114802-32-3 114802-34-5 114802-35-6
(catalyst and colorant, in transparent curable epoxy resins)
- RN 114802-32-3 HCAPLUS
- CN Iron, bis[4-methylbenzenesulfonic acid [1-(2-pyridinyl)ethylidene]hydrazidato]-, (T-4)- (9CI) (CA INDEX NAME)

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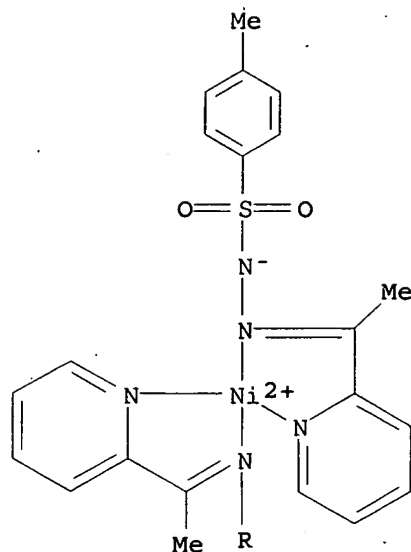


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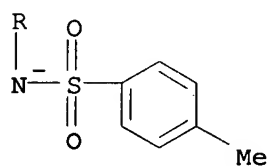


- RN 114802-34-5 HCAPLUS
- CN Nickel, bis[4-methylbenzenesulfonic acid [1-(2-pyridinyl)ethylidene]hydrazidato]-, (T-4)- (9CI) (CA INDEX NAME)

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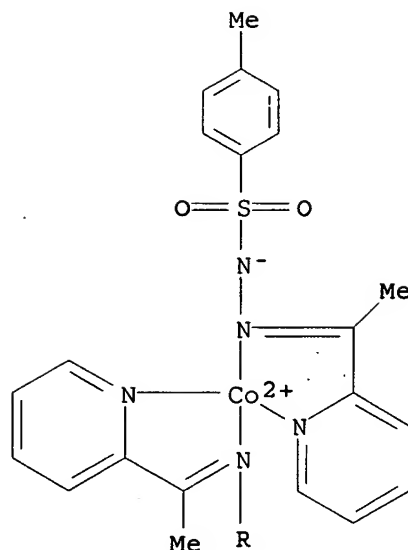


PAGE 2-A

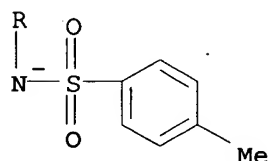


RN 114802-35-6 HCAPLUS
 CN Cobalt, bis[4-methylbenzenesulfonic acid [1-(2-pyridinyl)ethylidene]hydrazidato]-, (T-4)- (9CI) (CA INDEX NAME)

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- IC ICM C08G059-70
 CC 37-6 (Plastics Manufacture and Processing)
 Section cross-reference(s): 38
 ST epoxy curing **catalyst** colorant transparency; iron complex **catalyst** colorant epoxy; cobalt complex **catalyst** colorant epoxy; thio compd **catalyst** colorant epoxy; amino compd **catalyst** colorant epoxy; crosslinking **catalyst** colorant epoxy; optoelectronic epoxy **catalyst** colorant
 IT Crosslinking agents
 (amines, for epoxy resins containing **catalysts** and colorants)
 IT Transparent materials
 (epoxy resins, curing **catalysts** and colorants for, metal complexes as)
 IT Amines, uses
 (hardeners, for transparent epoxy resins containing **catalysts** and colorants)
 IT Coloring materials
 (metal complexes as **catalysts** and, in transparent epoxy resins)
 IT Crosslinking **catalysts**
 (metal complexes as colorants and, in transparent epoxy resins)
 IT Epoxy resins, miscellaneous

- (transparent curable compns. containing amine hardener and, catalysts and colorants for)
- IT Caulking compositions
Putty
(transparent epoxy resins for, curing catalysts and colorants in)
- IT Coordination compounds
(chelates, curing catalysts and colorants, in transparent epoxy resins)
- IT Electronics
(opto-, transparent epoxy resins for, curing catalysts and colorants for)
- IT 77417-86-8 105084-63-7 105085-15-2 114802-32-3
114802-34-5 114802-35-6 121164-24-7
148161-56-2
(catalyst and colorant, in transparent curable epoxy resins)
- IT 4589-12-2D, metal complexes 6361-95-1D, metal complexes
6503-26-0D, metal complexes 7439-89-6D, Iron, complexes with nitrogen- and sulfur-containing ligands 7440-02-0D, Nickel, complexes with nitrogen- and sulfur-containing ligands 7440-48-4D, Cobalt, complexes with nitrogen- and sulfur-containing ligands 19490-90-5D, Diphenyl-2-pyridylcarbinol, metal complexes 52776-76-8D, metal complexes 91181-34-9D, metal complexes 102817-82-3D, metal complexes 147394-90-9D, metal complexes 147394-91-0D, metal complexes 147394-92-1D, metal complexes 147394-93-2D, metal complexes 147583-81-1 147584-50-7D, metal complexes
(catalysts and colorants, in transparent curable epoxy resins)
- IT 25068-38-6, Bisphenol A-epichlorohydrin copolymer
(transparent curable compns. containing amine hardener and, catalysts and colorants for)

L28 ANSWER 16 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:612554 HCAPLUS

DOCUMENT NUMBER: 117:212554

TITLE: New homogeneous rhodium catalysts for the regioselective hydroboration of alkenes

AUTHOR(S): Westcott, Stephen A.; Blom, Henk P.; Marder, Todd B.; Baker, R. Thomas

CORPORATE SOURCE: Dep. Chem., Univ. Waterloo, Waterloo, ON, N2L 3G1, Can.

SOURCE: Journal of the American Chemical Society (1992), 114(23), 8863-9

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

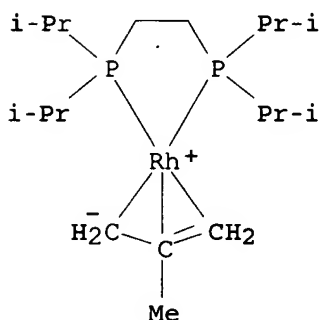
LANGUAGE: English

OTHER SOURCE(S): CASREACT 117:212554

AB Multinuclear (¹H, ¹¹B, ¹³C, ¹⁹F, and ³¹P) NMR spectroscopy was used to monitor primary products from transition metal-catalyzed addition of catecholborane (HBcat) to a variety of alkenes. Hydroboration of vinylarenes (indene, vinylanthracene, and XC₆H₄CH=CH₂, where X = p-OMe, p-F, p-Cl, and m-F) with HBcat, employing [Rh(η³-2-Me-allyl){(Me₂CH)₂PCH₂CH₂P(CHMe₂)₂}₂] (9) as catalyst precursor, proceeded with excellent activity and regioselectivity (>99%) in favor of the corresponding internal boronate ester. Analogous hydroboration reactions carried out in the presence of [Rh(COD){(Ph₂PCH₂CH₂)₂}]BF₄ (11, COD = 1,5-cyclooctadiene) or Wilkinson's catalyst, [RhCl(PPh₃)₃] (1),

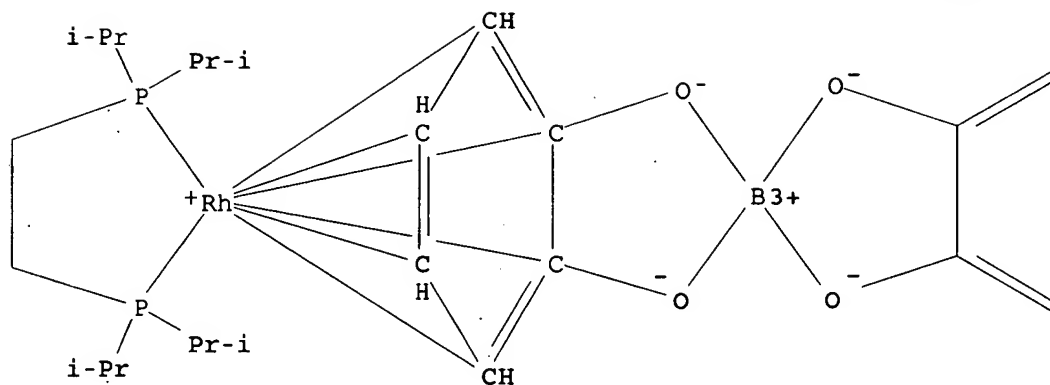
also gave internal boronate esters with regioselectivities comparable to those of 9. With 1, unlike 9 and 11, however, small amts. (ca. 5%) of hydrogenation products were observed consistently. With (E)-1-phenylpropene, 9 and 11 again gave internal boronate ester (>99%), whereas 1 gave a 70:30 mixture of internal:terminal boronate esters, with 5% propylbenzene as a side product. The effect of varying the chelating bis(phosphine) in $[\text{Rh}(\eta^3\text{-2-Me-allyl})(\text{P}2)]$ was examined for catalyzed hydroborations of 2-phenylpropene. Higher chemical yields and Markovnikov selectivities were observed for arylphosphines compared with corresponding bulky alkylphosphines. Unlike cationic $[\text{Rh}(\text{diene})(\text{P}2)]^+$ catalyst precursors, hydroborations of aliphatic alkenes using 9 proceeded with complete regiocontrol to give terminal alkylboronate esters. Hydroboration of 2,3-dimethylbut-2-ene with HBcat was also catalyzed by 9 and 11; complex 1 failed to catalyze hydroboration of this sterically demanding substrate. Complex 9 reacts with excess HBcat to form **zwitterionic** $[\text{Rh}(\eta^6\text{-catBcat})\{(\text{Me}_2\text{CH})_2\text{PCH}_2\text{CH}_2\text{P}(\text{CHMe}_2)\}_2]$, which is proposed to be the resting state of the active hydroboration catalyst. *in situ* monitoring of catalytic reactions using allylrhodium precursors by ^{31}P NMR spectroscopy showed that only the **zwitterionic** species were present in observable quantities at any time during or after completion of catalysis. Conversely, hydroborations using 11 gave several phosphinorhodium complexes, leading eventually to catalyst decomposition. The new **zwitterionic** catalysts can also be generated conveniently from $[\text{Rh}(\text{acac})(\eta\text{-C}_2\text{H}_4)_2]$ (acac = acetylacetonate), phosphine ligands, and HBcat.

IT 130641-61-1 134588-22-0 143969-50-0
(catalyst, for regioselective hydroboration of vinylarenes)
RN 130641-61-1 HCAPLUS
CN Rhodium, $[\text{1,2-ethanediy}[\text{bis}[\text{bis}(1\text{-methylethyl})\text{phosphine}]]\text{-P,P'}][(\text{1,2,3-}\eta)\text{-2-methyl-2-propenyl}]\text{- (9CI) (CA INDEX NAME)}$

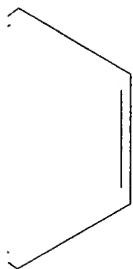


RN 134588-22-0 HCAPLUS
CN Rhodium, $[[\eta^6\text{-1,2-benzenediolato}(2-)-\kappa\text{O},\kappa\text{O}']][1,2\text{-benzenediolato}(2-)-\kappa\text{O},\kappa\text{O}']\text{borato}(1-)][1,2\text{-ethanediy}[\text{bis}[\text{bis}(1\text{-methylethyl})\text{phosphine-}\kappa\text{P}]]\text{- (9CI) (CA INDEX NAME)}$

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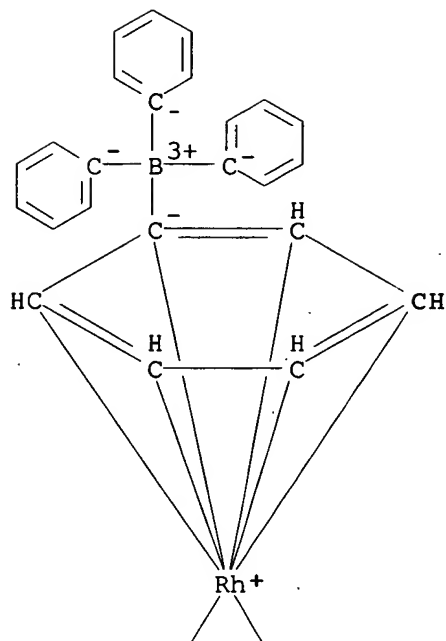


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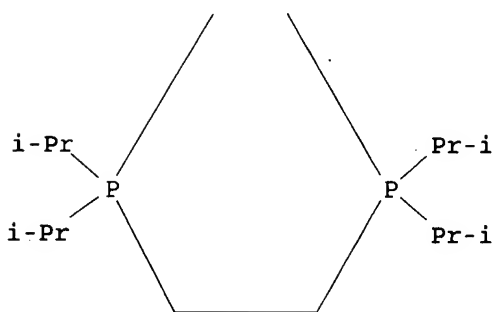


RN 143969-50-0 HCAPLUS
 CN Rhodium, [1,2-ethanediylbis[bis(1-methylethyl)phosphine-
 κ P]] [μ -(η : η 6-phenyl)] (triphenylboron) - (9CI) (CA
 INDEX NAME)

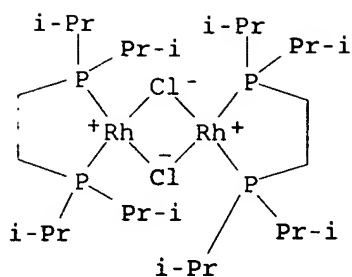
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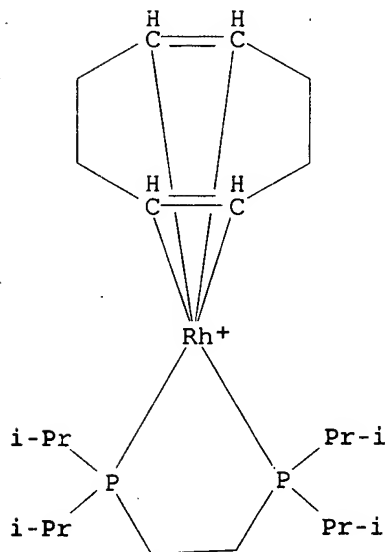
IT 107820-57-5 143969-48-6
 (preparation as catalyst, for regioselective hydroboration of
 vinylarenes)
 RN 107820-57-5 HCAPLUS
 CN Rhodium, di- μ -chlorobis[1,2-ethanediylbis[bis(1-
 methylethyl)phosphine- κ P]]di- (9CI) (CA INDEX NAME)



RN 143969-48-6 HCAPLUS
 CN Rhodium(1+), [(1,2,5,6- η)-1,5-cyclooctadiene] [1,2-ethanediylbis[bis(1-methylethyl)phosphine]-P,P']-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

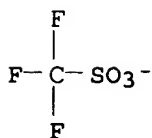
CM 1

CRN 143969-47-5
 CMF C22 H44 P2 Rh
 CCI CCS



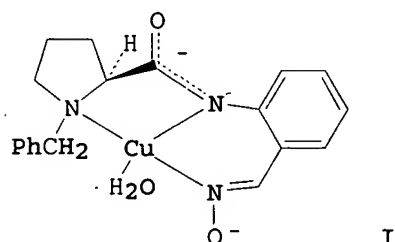
CM 2

CRN 37181-39-8
 CMF C F3 O3 S



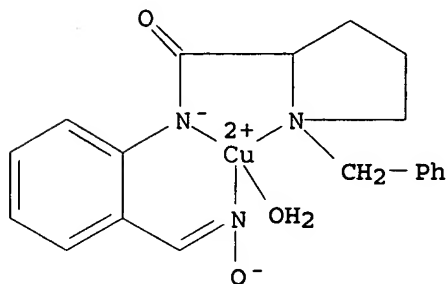
CC 29-4 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 23
 IT 14694-95-2 72332-27-5 72840-15-4 79255-71-3 81177-96-0
 130641-61-1 134588-22-0 143969-49-7
 143969-50-0
 (catalyst, for regioselective hydroboration of vinylarenes)
 IT 107820-57-5 143969-46-4 143969-48-6
 (preparation as catalyst, for regioselective hydroboration of vinylarenes)

L28 ANSWER 17 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1992:611767 HCAPLUS
 DOCUMENT NUMBER: 117:211767
 TITLE: The mechanism of hydrolysis of azlactones
 catalyzed by the copper(II) complex of
 (S)-2-[(N-benzylpropyl)amino]benzaldoxime
 AUTHOR(S): Belokon, Yu. N.; Bachurina, I. B.; Tararov, V.
 I.; Saporovskaya, M. B.
 CORPORATE SOURCE: A. N. Nesmeyanov Inst. Organoelem. Compd.,
 Moscow, 117813, Russia
 SOURCE: Izvestiya Akademi Nauk, Seriya Khimicheskaya
 (1992), (3), 536-46
 CODEN: IASKEA; ISSN: 0002-3353
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI



AB The spontaneous and the title complex (I)-catalyzed hydrolysis of 2-methyl-4-benzyl-5(4H)-oxazolone (MBA) was studied in H₂O-MeCN. I is an efficient catalyst for the hydrolysis (chymotrypsin is not effective). The hydrolysis involves formation of a substrate-catalyst complex in which MBA is coordinated with Cu via N(3). The rate-determining step involves attack of the oxime O at the iminic C(2) within the complex. The kinetic order with resp. to catalyst changes from one to one-half with increase in catalyst concentration; this suggests that I is present in aqueous solution in dimeric and monomeric forms and that only the monomeric form is responsible for the catalysis. An excess of MBA causes an inhibition of the hydrolysis; this is attributed to participation in the transition state of a water mol., coordinated in apical complex position, which is replaced by an excess of the substrate.
 IT 144234-30-0
 (catalysts, for hydrolysis of methylbenzyloxazolone)
 RN 144234-30-0 HCAPLUS

CN Copper, aqua [N-[2-[(hydroxyimino)methyl]phenyl]-1-(phenylmethyl)-2-pyrrolidinecarboxamidato(2-)-N1,N2,N2']-, [SP-4-4-(S)]- (9CI) (CA INDEX NAME)



CC 22-4 (Physical Organic Chemistry)
 Section cross-reference(s): 34
 ST mechanism hydrolysis methylbenzyloxazolone catalyst
 copper benzylprolylaminobenzaldoxime; oxazolone methylbenzyl
 hydrolysis catalyst mechanism; prolylaminobenzaldoxime
 catalyst hydrolysis methylbenzyloxazolone
 IT Hydrolysis catalysts
 ([(benzylprolyl) amino] benzaldoxime copper complex, for
 methylbenzyloxazolone)
 IT Transition state structure
 (in hydrolysis of methylbenzyloxazolone catalyzed by
 [(benzylprolyl) amino] benzaldoxime copper complex)
 IT 138191-67-0 144234-30-0
 (catalysts, for hydrolysis of methylbenzyloxazolone)
 IT 5469-44-3
 (hydrolysis of, mechanism of catalytic)

L28 ANSWER 18 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1990:532338 HCAPLUS

DOCUMENT NUMBER: 113:132338

TITLE: Reactivity of o-[(dimethylamino)methyl]phenol
 in reaction with p-nitrophenyl esters of
 phosphorus acids. Effect of copper(II) ions

AUTHOR(S): Ryzhkina, I. S.; Kudryavtseva, L. A.;
 Bel'skii, V. E.; Ismaev, I. E.; Morozov, V.
 I.; Il'yasov, A. V.; Ivanov, B. E.

CORPORATE SOURCE: Inst. Org. Fiz. Khim. im. Arbuzova, Kazan,
 USSR

SOURCE: Zhurnal Obshchei Khimii (1990), 60(4), 820-7
 CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal

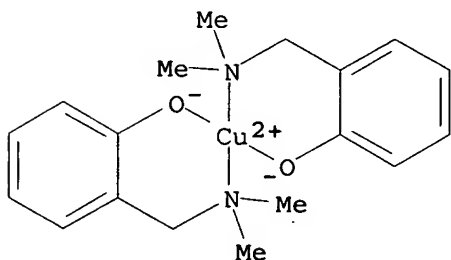
LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 113:132338

AB The kinetics of nucleophilic substitution reaction of
 RR1P(O)OC6H4NO2-p (I; R = R1 = CH2Cl; R = CH2Cl, R1 = OEt; R = R1
 = OPh) with o-[(Me2N)CH2]C6H4OH (II) was decomposed into
 contributions from protonated, zwitterionic, and
 thiolate forms of II. A bifunctional mechanism was put forward to
 rationalize the observation that the reactivity of the
 zwitterion increased, and of the phenolate decreased, with
 increasing number of P-O bonds in I. Complex [CuH·II]2+ was
 30-80 times more reactive in nucleophilic substitution/hydrolysis
 with I than [Cu·2II], reflecting the charge and

coordination degree of the former, and an order of magnitude more reactive than II phenolate; $[\text{CuH}\cdot\text{II}]^{2+}$ was also a substrate-specific catalyst, effective for I but ineffective for p-O₂NC₆H₄OAc.

- IT 98075-82-2
 (catalyst, for hydrolysis of phosphorus nitrophenyl esters)
 RN 98075-82-2 HCAPLUS
 CN Copper, bis[2-[(dimethylamino-κN)methyl]phenolato-κO]-
 (9CI) (CA INDEX NAME)



- CC 29-7 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 7, 22
 IT Tautomerization
 (of [(dimethylamino)methyl]phenol, equilibrium of zwitterion
 formation in)
 IT 98075-82-2
 (catalyst, for hydrolysis of phosphorus nitrophenyl esters)